Study on environmental and health effects of HFO refrigerants (Publication number: M-917|2017)

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Study on environmental and health effects of HFO refrigerants

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Disclaimer

The views and propositions expressed herein are, unless otherwise stated, those of Risk & Policy Analysts and do not necessarily represent any official view of the Norwegian Environment Agency or any other organisation mentioned in this report.

List of abbreviations

A2L	Mildly flammable refrigerants category
A5; non-A5	Article 5 Developing countries; non-Article 5 Developed countries
BAU	Business As Usual
Cefic	European Chemical Industry Council
$CF_3C(O)H$	Trifluoroacetaldehyde
CF_3COO^-	Trifluoroacetate
CFC	Chlorofluorocarbon
CLP	Classification, Labelling and Packaging
CMR	Carcinogenic, mutagenic or toxic to reproduction
CO_2	Carbon dioxide
COF_2	Carbonyl fluoride
CSR	Chemical Safety Report
EC_{10}	10% effective concentration (the concentration that causes the measured effect in 10% of organisms)
EC_{25}	25% effective concentration (the concentration that causes the measured effect in 25% of organisms)
EC_{50}	Half maximum response dose (the concentration that causes the measured effect in 50% of organisms)
ECHA	European Chemicals Agency
EEAP	Environmental Effects Assessment Panel
EUSES	European Union System for the Evaluation of Substances
GWP	Global Warming Potential
HC(O)Cl	Formyl chloride
HC(O)F	Formyl fluoride
HC(O)OH	Formic acid
HCFC	Hydrochlorofluorocarbon
HCFO	Hydrochlorofluoroolefin
HCHO	Formaldehyde

HCl	Hydrochloric acid
HF	Hydrofluoric acid, hydrogen fluoride
HFC	Hydrofluorocarbon
HFO	Hydrofluoroolefin
LC_{50}	Lethal concentration for 50% of the population
LOAEL	Local Observed Adverse Effect Level
MAC	Mobile Air Conditioning
MAK	Maximum Concentration at the Workplace
MIT-5	Mitigation 5
MoE	Margin of Exposure
MOS	Margin Of Safety
NO	Nitric oxide
NO_3	Nitrate radical
NOAEL	No Observed Adverse Effect Level
NOEC	No Observed Effect Concentration
NOEL	No Observed Effect Level
O_3	Ozone
ODS	Ozone-depleting substance
OECD	Organization for Economic Cooperation and Development
OEL	Occupational exposure level
OH	Hydroxyl radical
PEC	Predicted Environmental Concentration
PNEC	Predicted No-Effect Concentration
PPE	Personal Protection Equipment
ppm	Parts per million
ppt	Parts per trillion
QSAR	Quantitative Structure Activity Relationship
RAC	Refrigeration & Air Conditioning

RACHP	Refrigeration, Air Conditioning and Heat Pumps
RCR	Risk Characterisation Ratio
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SDS	Safety Data Sheet
SNAP	Significant New Alternatives Policy
STP	Sewage Treatment Plan
TEAP	Technology and Economic Assessment Panel
TFA	Trifluoroacetic acid, $CF_3C(O)OH$
TFF	Trifluoroacetyl fluoride, CF_3COF
TSCA	Toxic Substances Control Act
TWA	Time-weighted average
UNEP	United Nations Environment Programme
US EPA	United States Environmental Protection Agency
WMO	World Meteorological Organization

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Summary

This report describes the findings of a study on environmental and health effects of HFO (hydrofluoroolefin) refrigerants conducted for the Norwegian Environment Agency. The aim of the study were threefold, to identify the HFO substances used as refrigerants and their related emissions, and discuss the atmospheric dispersion, degradation and subsequent deposition of the degradation products. This was followed by an assessment of the environmental and human health impacts associated HFOs and their degradation products. Finally, a risk assessment was performed to assess how the future use of HFOs and their subsequent emissions would affect the environment globally up to 2100.

Information for the study was gathered from systematic search and review of the academic and grey literature. Consultation was also conducted with various stakeholders, including a manufacturer of HFO refrigerants, a company involved in the reclamation of HFO refrigerants, academic experts, a non-government organisation and a refrigeration industry association.

HFO substance information was collated from review of the literature, consultation and the patent database. A number of HFOs were identified as refrigerants that were commonly used, likely to be used in the future and those at different stages of development. HFO-1234yf is the most commonly used HFO substance as is a replacement for HFC-134a in mobile air-conditioning with HFO-1234ze and HFO-1233zd also being identified as being used as refrigerants. A number of HFO/HFC blends have also been identified as being used as refrigerants, such as R-448a with the main driving force for HFO blends being their lower global warming potential compared to pure HFCs. There are also other potential HFO substances that have been identified that may be used as refrigerants in the future such as HFO-1244yd and HFO-136mzz. HFO refrigerants are high in purity; however, there is limited information available on the identity of any impurities present.

Projected emissions of HFO refrigerants (HFO-1234yf) have also been calculated up to 2100 using BAU and MIT-5 scenarios, with emissions of HFOs and other low-GWP refrigerants expected to climb to 2050. With the addition of contributions from Article 5, these peak emissions could exceed 500,000 tonnes per year, although this will be need closer monitoring as the trends evolve. Emissions between 2050 and 2100 have been calculated using a plateau scenario (in 2100, emissions have been calculated to be over 339,000 tonnes) and a phase-out scenario (in 2100, emissions would be zero) using the MIT-5 scenario.

The final atmospheric degradation products of HFOs are dependent on the identity of the HFO. For example, the most commonly used HFO substance at present, HFO-1234yf, undergoes atmospheric degradation producing a 100% molar yield of trifluoroacetic acid, TFA. The degradation products of other HFOs are HF, HCl, formic acid and carbon dioxide in varying proportions.

In the atmosphere, a rapid partitioning of TFA into droplets of clouds, rain and fog occurs) with wet precipitation assumed to be the major source of TFA in the biosphere. TFA is found in a wide range of water bodies such as rivers, streams, lakes and wetlands where inflow into these water bodies occur from precipitation, glaciers, runoff from land, groundwater (springs) and water-treatment facilities where it forms trifluoroacetate salts ($CF3COO^-$) with minerals such as calcium and sodium. TFA concentrations in the environment vary with compartment and location with the highest concentrations witnessed in terminal water bodies such as salt lakes, playas and oceans. There have been few studies on TFA concentrations in groundwater to date but of the few studies that have been conducted, concentrations have been low. This is unexpected as TFA is poorly retained in soil and has large mobility, but may be due to the slow percolation into the groundwater samples that have been tested to date. In freshwaters, TFA is thought to be solely anthropogenic in nature; however, TFA found in oceans is both natural and anthropogenic in source.

Of the tested aquatic organisms, only the alga *R. subcapitata* displayed sensitivity to TFA, although this needs to be confirmed by retesting. However, there is no published data for toxicity to soil macroorganisms except arthropods, terrestrial arthropods or for to birds or soil microorganisms. There is less than satisfactory information on the toxicity of TFA and salts to terrestrial plants, and no studies have been reported for concentrations of TFA in crops for human consumption (Solomon et al. 2016). Furthermore, there is no information on toxicity to organisms found in salt lakes and playas. This is particularly important because salt lakes are the most likely site for accumulation of TFA in the natural environment. ECHA have highlighted the inadequacy and absence of toxicity data in the TFA REACH registration dossier and have instructed the lead registrant for the substance to address this by 2021. At present, however, the consensus amongst academic experts is that TFA will have a negligible effect on the environment.

A number of knowledge gaps need to be addressed to conclude that TFA will have negligible effect on the environment. Generally, more research is needed to fully understand the cycle of TFA in the atmosphere and hydrosphere. There is also a lack of information on the amounts of TFA used globally or other potential sources of TFA in the environment i.e. other chemicals with TFA as a degradation product.

The health hazards of HFO refrigerants have been investigated, in particular the health and safety of workers. There is limited information available in the literature on the health effects, with the health effects from material safety data sheets stating that HFOs are asphyxiant in high concentrations and that contact with the evaporating liquid may lead to freezing of the skin or frostbite. The REACH registration dossier for HFO-1234yf lists the substance to be low hazard for inhalation exposure, dermal exposure and eyes. No thresholds for the hazard have been identified. This registration dossier has been subject to an ECHA review with additional work identified to be performed. Refrigeration workers in the EU who handle HFO refrigerants are also subject to the requirements of the F gas regulations, whilst in manufacturing, exposure levels are generally between 0 and 1 ppm. For accident release or elevated levels of HFOs, a number of recommended measures have been identified and discussed. The main thermal decomposition products (dependent of HFO or HFO blend) are carbonyl fluoride; carbon oxides; carbon monoxide, hydrogen fluoride, carbonyl halides, hydrochloric acid and fluorocarbons.

A risk assessment was performed for HFO refrigerant use up to the 2100 which was based on the most commonly used HFO substance, HFO-1234yf, and its degradation product, TFA. The risk assessment was performed using EUSES and with a basic PEC:PNEC analysis also performed. The outcome of the risk assessment supported similar conclusions identified in literature, these being that toxicity risk of TFA to organisms and human health appears to be low, however, TFA is expected to become concentrated in terminal sinks due to TFA being highly persistent. The risk, therefore, increases if emissions of HFO-1234yf to the environment increase.

A number of knowledge gaps were identified during the study which may be addressed during any future studies. Many of these gaps concerned the toxicity data for TFA being inadequate or missing not allowing a thorough assessment of the effects this may have on the wider environment. For example, there is no information on toxicity to organisms found in salt lakes and playas which is important as these environmental compartments are terminal sinks for TFA. There have been few studies on TFA concentrations in groundwater and no measurements of the concentrations of TFA in crops for human consumption have been reported. ECHA have highlighted gaps and inadequacies in the toxicity data in the registration dossier for TFA for both the environment and human health, and have asked the lead substance registrant to address these in an updated dossier by 2021. The risk assessment performed for HFO refrigerants up to the 2100 could be repeated when the REACH registration dossier for TFA has been fully updated in 2021.

1 Introduction

1.1 Background

The Montreal Protocol on Substances that Deplete the Ozone Layer regulates the production and consumption of nearly 100 ozone depleting substances (ODS). The Protocol was adopted on 15th September 1987, and is the only UN treaty to date that has been ratified by all 197 UN Member States (United States EPA, 2016). The treaty has evolved over time considering new scientific, technical and economic developments, and it continues to be amended and adjusted. The latest amendment to the Protocol took place in Kigali, Rwanda in 2016 and introduced a phase-down schedule for HFCs (hydrofluorocarbons).

HFCs, used as refrigerants and in other applications (such as blowing agents), are potent greenhouse gases with a Global Warming Potential (GWP) up to five thousand times greater than carbon dioxide (NASA, 2015). An alternative to HFCs are the HFOs (hydrofluoroolefins), which have zero ozone depletion potential and low GWP. However, the final atmospheric HFO degradation products such as trifluoroacetic acid (TFA) and hydrofluoric acid (HF) may have environmental and human health effects (Wallington et al, 2014) which will be investigated in this study. For example, TFA is a highly persistent pollutant, with both anthropogenic and natural sources, and is ubiquitous in precipitation and ocean water even in remote areas (Hansen et al, 2015).

1.2 Objectives of the study

The objectives of the study are:

- To determine the HFO substances that are used or likely to be used as refrigerants, their related emissions, degradation products of HFOs and their atmospheric dispersion;
- To assess the environmental and health effects of HFOs and their degradation products; and
- To perform an assessment of how the future use of HFOs and their subsequent emissions would affect the environment globally.

1.3 Aims and structure of this report

The aim of this report is threefold. Firstly, it discusses the use of HFO refrigerants, their related emissions, atmospheric dispersion, degradation and the deposition of subsequent degradation products. This is followed by an assessment of the environmental and human health impacts associated HFOs and their degradation products. Finally, a risk assessment is performed to assess how the future use of HFOs and their subsequent emissions would affect the environment globally up to 2100.

The report is organised as follows:

- Section 2: Summarises the methodology employed for the study;
- Section 3: Provides HFO substance information;
- Section 4: Discusses HFO emissions;
- Section 5: Discusses the chemical processes and degradation products of HFOs;
- Section 6: Assessment of the environmental impacts of HFOs and their degradation products;
- Section 7: Assessment of the human health impacts of HFOs and their degradation products;
- Section 8: Discusses the outcomes of the risk assessment;

- Section 9: Discusses the conclusions of the study;
- Section 10: Recommends further work needed to address knowledge gaps;
- Section 11: Lists the references;
- Annex 1: Lists consultation questions;
- Annex 2: Detailed information about methodology;
- Annex 3: TFA VEGA output; and
- Annex 4: EUSES Summary 2025 and 2100 Plateau.

2 Methodology

2.1 Overview of the methodology

The methodology for the study has been divided into the following stages which are introduced below, and discussed in more detail in Annex 2.

- Task 1: Grey literature search;
- Task 2: Academic literature search;
- Task 3: Screening of the literature using DistillerSR®; and
- Task 4: Consultation

Additionally, the methodology employed for the calculation of the projected emissions and for the risk assessment of HFO refrigerants are introduced below, and discussed in more detail in Annex 2.

- Task 5: Project emissions up to 2100; and
- Task 6: Risk assessment up to 2100

For Tasks 5 and 6, the scenarios which have been modelled for post 2050 emissions are:

- Emissions are stabilised after 2050; or
- There is a phase-out of HFO refrigerants after 2050

2.2 Task 1: Grey literature

Relevant studies for the grey literature were identified from a comprehensive Google search and also a targeted search of relevant agencies, associations and manufacturers of refrigerants; these are detailed in Annex 2.

Additional grey literature was been searched based on consultation responses. The grey literature was screened for relevance and the relevant data extracted using DistillerSR®. Based on the outcome of one consultation, and after the literature review, the patent database was subsequently searched for impurity information.

2.3 Task 2: Academic literature

Based on the results obtained from searching the grey literature, the academic literature was reviewed for relevant studies. Search terms were developed in PubMed and are discussed in Annex 2. These search terms were broad in scope to ensure a wide range of relevant literature for HFO substance information, HFO emissions, chemical processes and degradation products, and environmental and human health impacts was retrieved. Google Scholar was also reviewed for relevant studies.

The academic literature was screened for relevance and the relevant data extracted using DistillerSR®, as discussed in Annex 2.

2.4 Task 3: Selection of relevance and data extraction- DistillerSR®

2.4.1 Screening of the literature

The literature identified during the grey literature and academic literature searches was scoped for relevance to the study. This is a two stage process based on templates created in DistillerSR® and described in detail in Annex 2.

2.4.2 Data extraction

For studies that were relevant after screening, the relevant data was extracted using DistillerSR®, this is described in detail in Annex 2.

2.4.3 Literature review outputs

The results of the grey and academic literature review for determining the HFO substances that are used or likely to be used as refrigerants, their related emissions, degradation products of HFOs and their atmospheric dispersion are described in detail in Figure 11-1 in Annex 2 and for the environmental and health effects of HFOs and their degradation products in Figure 11-2 in Annex 2.

2.5 Task 4: Consultation

Eight stakeholders were contacted for consultation for the study. These included academic experts, a non-government organisation, a HFO refrigerant manufacturer, a HFO refrigerant reclaimer and a refrigeration industry association. Questions asked during the consultations are listed in Annex 1.

2.6 Task 5: Assessing HFO projections

2.6.1 Introduction

The TEAP Task Force Report (XXVII/4) from September 2016 is the most appropriate source for calculating HFO emissions. This was the final TEAP report leading into the Kigali negotiations. The report provides valuable consumption information that we can convert through existing modelling techniques into emission estimates.

The report contains tabulated projected consumption by refrigerant category and RAC (Refrigeration & Air Conditioning) sub-sector in 5 year intervals. From this, it is possible to interpolate for the intervening years and build-up a picture of growth of HFO use, subject to the following:

- Annex 4 only records low-GWP refrigerants as a category, so this would include CO_2, ammonia and hydrocarbons, as well as HFOs;
- Table 2-7 indicates that low-GWP in the terms of the Report means <300 GWP; and
- Tables 2-3 & 2-4 give various pure substances and blends that could qualify.

Annex 4 of the TEAP report also maps at least two Mitigation Scenarios which could be followed in terms of likely low-GWP (Mitigation 5 scenario (MIT-5) and Business As Usual (BAU)). MIT-5 assumes the completion of conversion of key non-Article 5 RAC equipment by 2025 and the commencement of similar conversions in Article 5 countries by the same date.

MIT-5 was viewed as the most representative scenario in respect of the Kigali Amendment that eventually emerged, although even this was marginally too aggressive. However, an over-aggressive schedule would inflate the consumption and emissions of low-GWP alternatives such as HFOs and thereby make the environmental risk assessment appropriately conservative by over-stating consumption and resulting emissions.

2.7 Task 6: Risk assessment for HFOs

Approach to Assessment

This risk assessment has considered the exposure of the environment to TFA, including the basis for determining the exposure of humans via the environment. Although there is a range of HFO compounds used in the EU, this risk assessment considers the main breakdown product TFA. Although additional exposure assessments could be conducted, encompassing the use of the various other products and their breakdown products, it is anticipated that the assessment of TFA will provide a worst case assessment.

The methodology used for the risk assessment is as follows using EUSES:

- Estimate overall emissions by industry sector (organotin production, glass coating, stabilisers, catalysts and biocides);
- For each sector, estimate emissions by TFA and life-cycle stage (for example, emissions of TFA from different sources); and
- Determine the Predicted Environmental Concentrations (PECs) at a regional level for each of the TFA compounds using the EUSES model.

Further information on the inputs for the risk assessment model is discussed in Section 8.

2.7.1 VEGA

The VEGA platform has been employed to access the QSAR (Quantitative Structure Activity Relationship) models for TFA. The use of QSAR models allows the prediction of the properties of a substance from its structure (VEGA Hub, undated). For TFA, this has been used to examine the mutagenicity, carcinogenicity, development toxicity, fish toxicity, daphnia toxicity, and persistence. Other QSAR models can be used to predict the properties of TFA.

2.7.2 EUSES

The EUSES (European Union System for the Evaluation of Substances) software has been employed for assessing the environmental and human risks from HFO emissions (EU Science Hub, 2016). The EUSES model generates predicted environmental concentrations (PECs) from estimated releases from use patterns (based on emissions, which is further discussed in section 3) and substance properties (further discussed in Section 4). However, modelling of fluorinated compounds has been challenging. In this assessment a number of challenges were also identified, the calculated values should be used with caution.

3 Substance information

3.1 Overview of HFOs and HFO blends currently used/likely to be used as refrigerants

In the table below are the HFOs and HFO/HFC blends identified that are currently being used, likely to be used in the future, or have shown early promise but no longer being developed.

Table 3-1: HFOs and HFO/HFC blends currently used/likely to be used as refrigerants	
HFO	**Other known nomenclature**
HFO-1234yf	Solstice® yf Refrigerant, R-1234yf, 1234yf, HFC-1234yf, Opteon™ YF
HFO-1234ze	Solstice® ze, HFO-1234ze(E)
HFO-1233zd	Solstice® zd, HFO-1233zd(E), HCFO-1233zd
HFO-1224yd	Amolea® 1224yd, HFO-1224yd(Z)
HFO-1336mzz	Opteon™ 1100, HFO-1336mzz-Z, HFO-1336mzz(Z)
HFO-1243zf	-
HFO-1114	-
HFO-1216	-
HFO-1345czf	-
HFO-1123	-
HFO-1225ye(Z)*	-
HFO-1243z*	-
*Had early expectations, however, due to unforeseen toxicity data they are no longer favourable	
HFO/HFC blend	**Tradenames**
R-448A (HFO/HFC blend)	Solstice® N40 (R-448A)
R-449A (HFO/HFC blend)	Opteon™ XP40 (R-449A)
R-450A (HFO/HFC blend)	Solstice® N13 (R-450A)
R-452A (HFO/HFC blend)	Opteon™ XP44 (R-452A)
R-514A (HFO/other substance blend)	Opteon ™ XP30 (R-514A)
Manufacturer: Solstice® (Honeywell); Opteon™ (Chemours); Amolea®(Ashai Glass)	

Potential issue – inconsistent nomenclature use

HFOs can be referred to by a variety of nomenclature in the literature which can pose a challenge for a non-technical audience. For example, HFO-1234yf has been referred to as HFC-1234yf and R-1234yf. This is addressed in the following section where other known nomenclature for individual HFOs is stated.

There is also a potential issue for the naming of HFOs. HCFOs have been included in this study, as they are considered to be equivalent to HFOs as they are not listed under the Montreal Protocol or EU ODS regulations, and are listed under Annex II of the REACH regulation. However, there are many chlorinated substances with short atmospheric lifetimes that are not included under the Montreal Protocol, but this is subject to periodic review (e.g. in the case of methylene chloride).

3.2 HFO substances that are used/likely to be used as refrigerants

3.2.1 HFO only refrigerants

HFO-1234yf

HFO-1234yf ($C_3H_2F_4$) has been identified from literature review and consultation as the most widely used HFO refrigerant. HFO-1234yf is commonly being used as a replacement for HFC-134a in mobile air conditioning and is being rolled out as a 4th generation refrigerant.

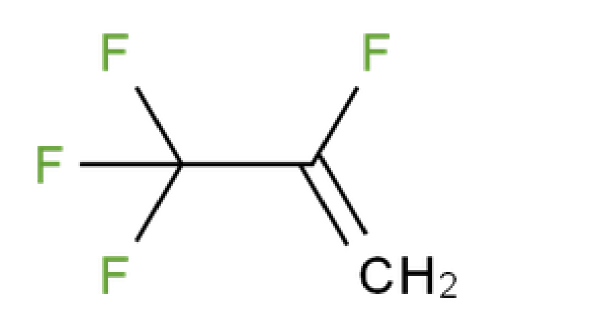


Figure 3-1: Chemical structure of HFO-1234yf Source: Chembase (2014): 2,3,3,3-tetrafluoroprop-1-ene. Available at: http://en.chembase.cn/molecule-8052.html

HFO-1234yf has been registered under REACH (ECHA, 2017a) under the name polyhaloalkene and 2,3,3,3-tetrafluoroprop-1-ene (CAS No. 754-12-1; EC No. 468-710-7/616-220-0) and is manufactured and/or imported in the European Economic Area in the tonnage range of 1,000 - 10,000 tonnes per year. The trade names Opteon™ YF and Opteon™ YF Aftermarket (see Table 3-1) are also registered under the ECHA registration (ECHA, 2017a).

Table 3-2: HFO-1234yf ECHA summary				
HFO substance	**Chemical formula**	**Tonnage registration (tonnes)**	**Other known nomenclature**	**REACH registrants**
HFO-1234yf, 2,3,3,3-tetrafluoroprop-1-ene	$C_3H_2F_4$; $CF_3CF=CH_2$	1,000 - 10,000	Solstice® yf Refrigerant (Honeywell); R-1234yf; 1234yf; HFC-1234yf; Opteon™ YF (Chemours)	Arkema France, Chemical Inspection and Regulatory Services; Chemours Netherlands B.V.; Honeywell Belgium; Honeywell Fluorine Products Europe; SCAS Europe S.A/NV
Sources: Arkema (2015): Industrial Specialities at a Glance 2014. Available at: https://www.arkema.com/export/sites/global/.content/medias/downloads/investorrelations/en/finance/Arkema_CMD_2015_MS_-Industrial_Specialties_Final_Version-v16.pdf Chemours (2017): Opteon™ YF Automotive Refrigerant. Available at: https://www.chemours.com/Refrigerants/en_US/uses_apps/automotive_ac/SmartAutoAC/HFO-1234yf.html ECHA (2017): Polyhaloalkene registration dossier. Available at https://www.echa.europa.eu/web/guest/registration-dossier/-/registered-dossier/16012 Honeywell (2017): Solstice® yf Refrigerant (R-1234y). Available at: http://msds-resource.honeywell.com/ehswww/hon/result/result_single_main.jsp?C001=MSDS&C102=GB&C101=SDS_GB&C100=E&P_LANGU=E&C013=&C997=C100;E%2BC101;SDS_GB%2BC102;GB%2B1000&P_SYS=1&C008=&C006=HON&C005=000000011078&				

It has also been registered by the US EPA under the Toxic Substances Control Act (TSCA). Production volumes were recorded as 126,760 lbs in 2011 but information has been withheld in the years 2012-2015 due to confidentiality reasons (Table 3-2). From consultation, the worldwide tonnage per region is confidential, however production is in the 10,000s tonnes range.

Table 3-3: HFO-1234yf US EPA summary			
HFO substance	**Chemical formula**	**National aggregate production volumes (pounds)**	**EPA registrants**
HFO-1234yf, 2,3,3,3-tetrafluoroprop-1-ene	$C_3H_2F_4$, $CF_3CF=CH_2$	2015-2012: data withheld 2011: 126,760 lbs	Honeywell International Inc; The Chemours Company
Sources: Chemical Data Reporting (CDR). Available at: https://java.epa.gov/chemview#dashboard			

HFO-1234ze

HFO-1234ze ($C_3H_2F_4$) has also been identified as being used as a refrigerant from literature review. HFO-1234ze is registered under REACH (EC No. 471-480-0) and is manufactured and/or imported in 100 - 1,000 tonnes per year (ECHA, 2017b).

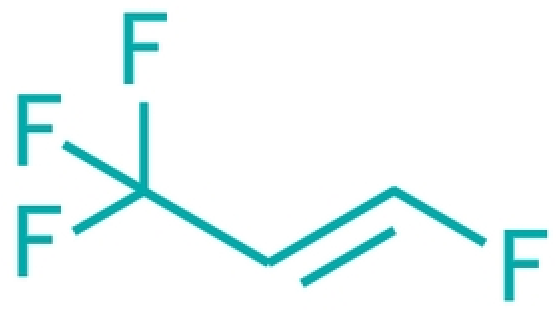


Figure 3-2: Structure of HFO-1234ze
Source: American Chemical Society (2017): Patent Picks: New Propellant Technologies. Available at: http://cen.acs.org/articles/93/i47/Patent-Picks-New-Propellant-Technologies.html

Table 3-4: HFO-1234ze ECHA summary

HFO substance	Chemical formula	Tonnage registration (tonnes)	Other known nomenclature	REACH registrants
HFO-1234ze, (E)-1,3,3,3-tetrafluoroprop-1-ene	$C_3H_2F_4$; (E)-$CF_3CH=CFH$	100 - 1,000	Solstice® ze (Honeywell); HFO-1234ze(E); R-1234ze	Information not publicly available
Sources: ECHA (2017): HFO-1234ze Substance Information. Available at: https://www.echa.europa.eu/web/guest/substance-information/-/substanceinfo/100.104.972?_disssubsinfo_WAR_disssubsinfoportlet_backURL=https%3A%2F%2Fwww.echa.europa.eu%2Fweb%2Fguest%2Fhome%3Fp_p_id%3Ddisssimplesearchhomepage_WAR_disssearchportlet%26p_p_lifecycle%3D0%26p_p_state%3Dnormal%26p_p_mode%3Dview%26p_p_col_id%3Dcolumn-2%26p_p_col_pos%3D1%26p_p_col_count%3D7%26_disssimplesearchhomepage_WAR_disssearchportlet_sessionCriteriaId%3D				

HFO-1234ze has not been registered by the US EPA under the Toxic Substances Control Act (TSCA).

HCFO-1233zd (HFO-1233zd)

HCFO-1233zd (which is also used as a blowing agent) has also been identified as being used in refrigerants from consultation. HCFO-1233zd is registered under REACH (CAS No. 102687-65-0; EC No. 700-486-0) and is manufactured and/or imported in 100 - 1,000 tonnes per year (ECHA, 2017b). It is worth noting, that this substance contains both fluorine and chlorine. HCFO-1233zd is referred to as an HFO as it is not listed under the Montreal Protocol or EU ODS Regulations; it is listed under Annex II of the EU F-Gas regulation. It will be referred to as HFO-1233zd herein.

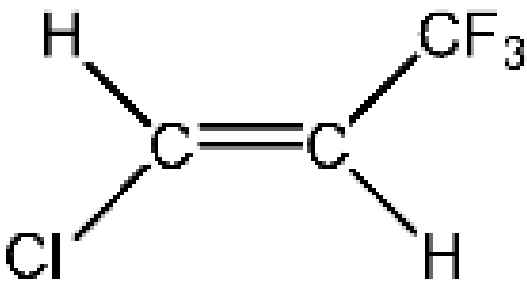


Figure 3-3: Structure of HFO-1233zd
Source: Patent application WO2011112339 A2. Catalyst life improvement for the vapour phase manufacture of 1-chloro-3,3,3-trifluoropropene. Available at: https://www.google.com/patents/WO2011112339A2

Table 3-5: HFO-1233zd ECHA summary

HFO substance	Chemical formula	Tonnage registration (tonnes)	Other known nomenclature	REACH registrants
HFO-1233zd, (E)-1-chloro-3,3,3-trifluoroprop-1-ene	$C_3H_2F_3Cl$; (E)-$CHCl{=}CHCF_3$	100 - 1,000	Solstice® zd (Honeywell); HFO-1233zd(E); R-1233zd; Solstice® LBA (blowing agent)	Arkema France; Honeywell Belgium; Honeywell Fluorine Products Europe
Sources: ECHA (2017): HCFO-1234zd Substance Information. Available at: https://echa.europa.eu/substance-information/-/substanceinfo/100.149.148 Honeywell Refrigerants (2017): Solstice® zd. Available at https://www.honeywell-refrigerants.com/americas/product/solstice-zd/				

It has also been registered by the US EPA under the Toxic Substances Control Act (TSCA). Production volumes have increased since 2012 with volumes in 2015 recorded in the range of 1,000,000 - 10, 000,000 lbs.

Table 3-6: HFO-1233zd US EPA summary

HFO substance	Chemical formula	National aggregate production volumes (pounds)	EPA registrants
HFO-1233zd, (E)-1-chloro-3,3,3-trifluoroprop-1-ene	$C_3H_2F_3Cl$; (E)-$CHCl{=}CHCF_3$	2015: 1,000,000 - 10,000,000 lbs 2014: 1,000,000 - 10,000,000 lbs 2013: <25,000 lbs 2012: <25,000 lbs	Honeywell International Inc
Source: Chemical Data Reporting (CDR). Available at: https://java.epa.gov/chemview#dashboard			

HFO-1224yd

HFCO-1224yd has been identified as being used in refrigerants from consultation. There is very limited information on this HFO and no EC or CAS number is available; only Ashai Glass (Japan) manufactures this HFO. According to the technical information from Ashai Glass (Ashai Glass, 2017) this HFO has a GWP <1 and its physical properties are very close to HFC-245fa.

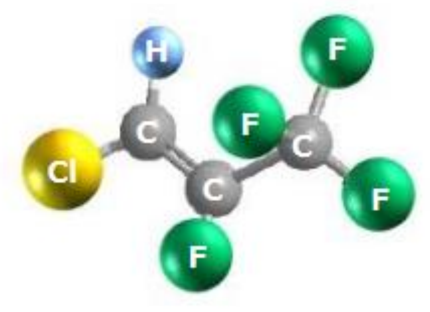


Figure 3-4: Structure of HFO-1244yd
Source: Ashai Glass (2017): Amolea® 1224yd Technical Information. Available at: http://www.agc-chemicals.com/file/AMOLEAyd_Tech_English_C.PDF

Table 3-7: HFO-1224yd summary

HFO substance	Chemical formula	Other known nomenclature	Manufacturers
HFO-1224yd, (Z)-2,3,3,3-tetrafluoro-1-chloroprop-1-ene	C_5F_4HCl; (Z)-$CHCl{=}CF{-}CF_3$	Amolea® 1224yd (Ashai Glass); HFO-1224yd(Z)	Ashai Glass

Source: Ashai Glass (2017): Amolea® 1224yd Technical Information. Available at: http://www.agc-chemicals.com/file/AMOLEAyd_Tech_English_C.PDF

Other HFO substances that are used or likely to be used as refrigerants

From literature review, a number of other HFO substances have been identified with the potential to be used as refrigerants which are summarised in the table overleaf. Two potential HFOs, 1225ye(Z) and 1243z had early expectations; however, due to unforeseen toxicity data they are no longer favourable (Calm et al, 2012).

Table 3-8: Other HFO substances that are used or likely to be used as refrigerants			
HFO substance	**Chemical formula**	**Other nomenclature**	**Refrigeration use**
HFO-1336mzz	$CF_3CH=CHCF_3$	Opteon™ 1100 (Chemours); HFO-1336mzz-Z; HFO-1336mzz(Z)	May be used as a refrigerant on its own from consultation. Used as a blend (see Table 3-8)
HFO-1243zf	$CF_3CH=CH_2$	N/A	May be used, however there may be toxicity issues
HFO-1114	$CF_2=CH_2$	N/A	May be used
HFO-1216	$CF_3CF=CF_2$	N/A	May be used
HFO-1345czf	$CF_3CF_2CH=CH_2$	N/A	May be used
Sources: Allgood (2015): New Generation of HFO refrigerants. Energy & Store Development Conference. Available at: https://www.chemours.com/Refrigerants/en_US/products/Opteon/Stationary_Refrigeration/assets/downloads/news/new-generation-hfo-refrigerants.pdf Raabe et al (2012): Molecular modelling of fluoropropene refrigerants. J Phys. Chem. B., 116, pp 5744-5751 RAC (2014): DuPont has high hopes for new non-flammable refrigerant HFO 1336mzz. Available at: https://www.racplus.com/news/dupont-has-high-hopes-for-new-non-flammable-refrigerant-hfo-1336mzz/8669689.article World Meteorological Organisation (2010). Global Ozone Research and Monitoring Project—Report No. 52. Scientific Assessment of Ozone Depletion: 2010. World Meteorological Organization, National Oceanic and Atmospheric Administration, National Aeronautics and Space Administration, United Nations Environment Programme and the European Commission. Available at: https://www.wmo.int/pages/prog/arep/gaw/ozone_2010/documents/Ozone-Assessment-2010-complete.pdf			

From consultation, HFO-1123 may also be used as a refrigerant. Ashai Glass were working on a refrigerant blend containing HFO-1123, however no more information is publically available (Ashai Glass, 2014).

3.2.2 HFO blends

Blends containing HFOs have been identified from literature review as being used or likely to be used as refrigerants. These blends typically consist of HFOs and HFCs and those that have been identified are described in Table 3-8. Consultation has identified the key features of HFO blends which are discussed below.

The main driving force for HFO blends are their lower GWPs in comparison to pure HFCs. HFO blends are also used due to the advantages of pressure range, have a specific hot gas temperature, and are also less flammable than pure HFO substances (although this is not a major factor compared with the lower GWP due to the C=C double bond). Compared to HFO/HFC blends, pure HFO substances are also harder to manufacture and are also more costly.

HFO blends R-448A, R-449A, R-450A and R-452A are commercially available with R-448 and R-449 being the most widely used.[1] There is also on-going research into blends, so the outlook and the blends available are continually evolving.

[1] Blends of HFO/HFC or other substance are often referred to by 'R' which simply means refrigerant followed by a number depending on the nature of the blend. The 'A' after the number refers to it being a zeotropic blend.

Table 3-9: HFO blends that are used as refrigerants		
HFO/HFC blend	Technical specifications	Tradenames
R-448A (HFO/HFC blend)	Honeywell Solstice® N40: 26% HFC-32, 26% HFC-125, 21% HFC-134a, 7% HFO-1234ze, 20% HFO-1234yf	Solstice® N40 (R-448A)
R-449A (HFO/HFC blend)	Chemours Opteon™ XP40: HFC-134a 25.7 wt%, HFC-1234yf 25.3 wt%, HFC-125 24.7 wt%, HFC-32 24.3 wt%	Opteon™ XP40 (R449A)
R-450A (HFO/HFC blend)	Honeywell Solstice® N13: 42% HFC-134a and 58% HFO-1234ze	Solstice® N13 (R-450A)
R-452A (HFO/HFC blend)	Chemours Opteon™ XP44: HFC-32 11.0 wt%, HFC-125 59.0 wt%, HFO-1234yf 30.0 wt.%	Opteon™ XP44 (R-452A)
R-514A (HFO/other substance blend)	Chemours Opteon™ XP30: HFO-1336mzz(Z) 74.7 wt.%, trans-1-2-dichloroethylene 25.3 wt.%	Opteon ™ XP30 (R-514A)
Sources: Climalife (2017): R-448A. Available at: http://climalife.dehon.com/uploads/product/media/document/r-448a-fd-en-17.pdf Chemours (2016): Opteon™ XP40. Available at: https://www.chemours.com/Refrigerants/en_US/products/Opteon/Stationary_Refrigeration/assets/downloads/Opteon-XP40-R-404A-R-507-retrofit-guidelines.pdf Honeywell (2017): Safety Data Sheet Honeywell Solstice® N13 Refrigerant (R-450A). Available at: https://msds-resource.honeywell.com/ehswww/hon/result/result_single.jsp?P_LANGU=E&P_SYS=1&C001=MSDS&C997=C100%3BE%2BC101%3BSDS_GB%2BC102%3BGB%2B1000&C100=*&C101=*&C102=*&C005=000000016417&C008=&C006=HON&C013=+ Chemours (2017): Safety Data Sheet Opteon™ XP44 (R-452A) Refrigerant. Available at: https://www.3eonline.com/ImageServer/NewPdf/f27c114b-a3d0-496c-b514-cdf8fd0c29da/0123abfa-fad2-4dc9-b173-e9d4e5fae816.pdf Chemours (2016): Opteon™ XP30 (R-514A) Refrigerant. Available at https://www.chemours.com/Refrigerants/en_US/products/Opteon/Stationary_Refrigeration/assets/downloads/opteon-xp30-product-information.pdf United Nations Environmental Program (2016): Lower-GWP Alternatives in Commercial and Transport Refrigeration: An expanded compilation of propane, CO2, ammonia and HFO case studies. Available at: http://wedocs.unep.org/handle/20.500.11822/14880		

3.3 HFO impurities

Consultation with an academic suggested that refrigerants are expected to have high purity and any impurities present are likely to be other HFCs or HFOs. The important issue of potential impurity release from factories that produce HFOs and the associated worker exposure and wider environmental implications was also raised during this consultation.

Honeywell have indicated in their published literature that contamination of HFO-1234yf systems with very low levels of HFC-134a and HFO-1225ye(Z) and unspecified fluorinated unsaturated alkene is an issue. Honeywell recommends maintaining the generic 40 ppm limit for cumulative fluorinated unsaturated alkene impurities, and a limit of 150 ppm for HFO-1225yeZ (Seeton and Wilson, 2010). Further consultation with a manufacturer, indicated that under classification and labelling requirements manufacturers have to label any classified impurity that exceeds 1000 ppm. If there is a CMR impurity present >1000 ppm then the substance has to be identified and labelled. They indicated that the total impurities present in their products are <2000 ppm with the majority being unreacted feedstock.

Overall, there is very little information about the identity of impurities in the academic literature and industry literature, however, some insight is given in a published patent. This patent relates to methods for removing halogenated ethylene impurities included in 2,3,3,3-tetrafluoro-1-propene (HFO-1234yf), 1,3,3,3-tetrafluoro-1-propene (HFO-1234ze) and 1-chloro-3,3,3-trifluoro-1-propene (HFO-1233zd). The inventors unexpectedly found that the final HFO-1234yf, HFO-1234ze and HCFO-1233zd products, which were obtained after the distillation of the aforementioned crude products, still contained halogenated ethylene impurities. For example, HFO-1234yf obtained after the dehydrochlorination step contained halogenated ethylene impurities such as HFO-1141 (CH_2=CHF), HCFO-1140 (CH_2=CHCl), and HCFO-1131 (CH_2=CFCl and/or trans/cis-CHF=CHCl). These halogenated ethylene impurities can be present in the product stream in an amount as much as 0.1% by weight, thereby reducing the concentration and purity. Moreover, it is well known that HCFO-1140 is a carcinogenic agent and the toxicity of other halogenated ethylenes is unknown. From a toxicity perspective, it is undesirable for these halogenated ethylenes to be present in the HFO-1234yf final product. In addition, the presence of these halogenated ethylenes may cause detrimental impact on the efficiency of the production of HFOs, such as HFO-1234yf, HFO-1234ze and HCFO-1233zd. Therefore, there is a need for means by which these unsaturated impurities can be removed or at least reduced from the HFO-1234yf product (United States Patent, Wang and Tung, 2016).

At present, other perfluorinated compounds like PFOS (perfluorooctanesulfonic acid) and PFOA (perfluorooctanoic acid) have not been identified as impurities from the literature review and consultation. Furthermore, consultation with a major manufacturer stated PFOS and PFOA cannot be generated from the raw materials (chemically impossible) or any processes used during the manufacture of HFOs. No information about the possible presence of PFBA in HFOs is publically available. This is the same case for HFO/HFC blends which also have a high level of purity.

4 HFO emissions estimates - projected up to 2100

4.1 Overview

This section describes the projected emissions of HFO refrigerants in non-Article 5 and Article 5 countries up to 2100. MAC (mobile air conditioning) has the biggest emissions with HFO-1234yf only used in this sector; so for emissions it has been assumed that all HFO emissions will results in TFA (trifluoroacetic acid). It should be noted, that not all HFOs breakdown to only TFA. Two approaches for emissions have been calculated, the BAU scenario and MIT-5.

4.2 Projected emissions

In the project brief, the sponsors of the project wished to see projected emissions through to 2100. This created a challenge in that consumption could not be reliably forecasted by TEAP beyond 2050. To deal with this, the authors, in conjunction with the sponsors, decided that two scenarios should be modelled to characterise the post-2050 emissions options. The first was to consider an abrupt phase-out of HFOs in the RAC sector at 2050 *(the phase-out scenario)*, thereby leaving any remaining emissions to emanate from the bank of installed refrigerant over the period until the sequential decommissioning took place at end-of-life. This was viewed as delivering the least 'supply' of HFO emissions into the environment while maintaining consistency with the TEAP data. The second option was to freeze the consumption of HFOs into new equipment at the 2050 level for the next 50 years *(the plateau scenario)*. This was seen as a relatively conservative assumption, since forecasting the acceptability of such a technology over such a long period is always fraught with uncertainty. Equally, any forecast of on-going growth in consumption from 2050 would be speculative and unfounded. Therefore, these two options were seen as realistic 'bounds' for the model.

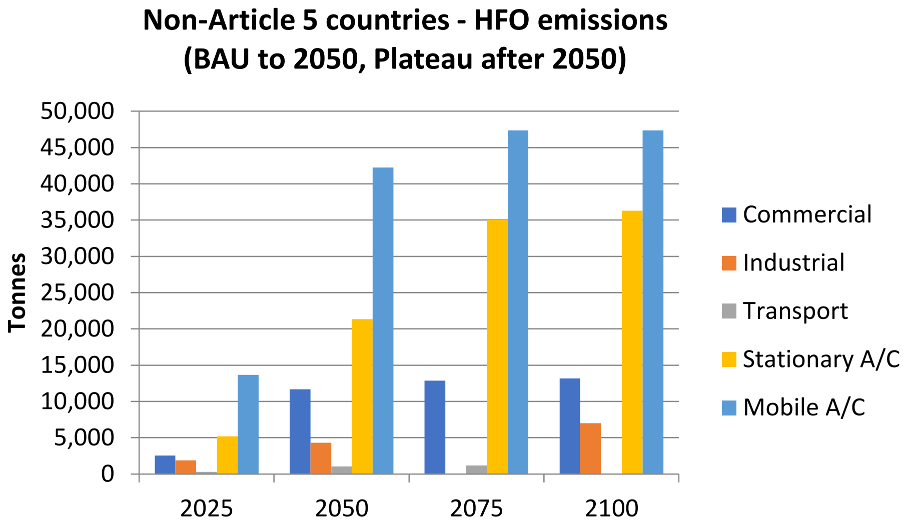
In determining the decline in the installed bank of equipment, it was also important to assign average life expectancies to each equipment type. Again, this was something partially addressed in the 2006 IPCC Emissions Reporting Guidelines, but expert judgement was viewed to be more appropriate owing to the passage of time.

4.2.1 Output from BAU scenarios up to 2050

The following table provides the form of output from the model for the non-A5 Business As Usual case:

Table 4-1: Non-Article 5 countries - HFO emissions (BAU up to 2050)								
					HFO Annual Emissions (tonnes)			
Scenario	Sector	Equipment Life (years)	HFO Allocation (%)	Emissions Rate/year (%)	2025	2050	2075	2100
Plateau after 2050	Commercial	30	50	15	2,533	11,696	12,882	13,172
	Industrial	30	20	10	1,902	4,318	6.911	7,001
	Transport	15	50	30	321	1,052	1,187	1.187
	Stationary A/C	30	50	25	5,218	21,354	35,040	36,311
	Mobile A/C	15	50	35	13,676	42,256	47,376	47,376
	Total				**23,650**	**80,677**	**103,396**	**105,047**
Phase-out after 2050	Commercial	30	50	15	2,533	11,696	2,260	0
	Industrial	30	20	10	1,902	4,318	1,265	0
	Transport	15	50	30	321	1,052	0	0
	Stationary A/C	30	50	25	5,218	21,354	5,756	0
	Mobile A/C	15	50	35	13,676	42,256	0	0
	Total				**23,650**	**80,677**	**9,281**	**0**

Graphical representations of the data in the table above are provided in the following figure:



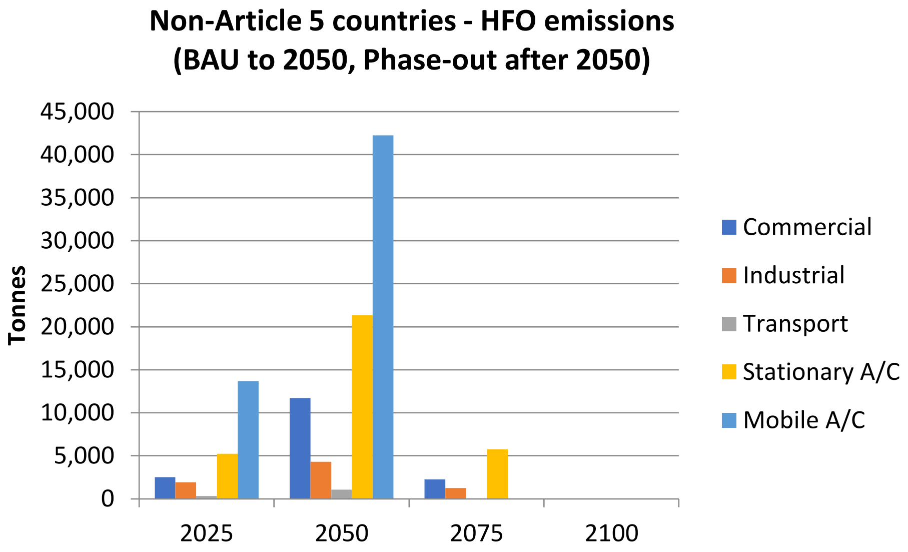


Figure 4-1: Non-Article 5 countries - HFO emissions (BAU), plateau (top graph) and phase-out (bottom graph) after 2050

Since the TEAP data only differentiated low-GWP refrigerants in the relevant tables, the authors needed to make a further assessment of likely use of HFOs as part of the low-GWP 'mix'. For example, in the Industrial Refrigeration sector, it was expected that ammonia would be quite a dominant low-GWP refrigerant and that HFOs, based largely on cost and efficiency, would be less prevalent (in this case assumed at 20%). However, in other areas, the convenience of HFOs would likely make them more popular, especially if charge sizes could be reduced without sacrificing efficiency. Under these circumstances, a default allocation of 50% was given, although these values can be adjusted in the model for sensitivity purposes.

For Table 4-1 and Figure 4-1, only contributions for non-Article 5 chave been calculated. This has been used to show the example of the data contained within the TEAP report and how this data can be applied for calculating HFO emissions.

4.2.2 Output from MIT-5 scenarios up to 2050

The outputs for the MIT-5 scenario were seen as most relevant to this work for the reasons cited earlier (Section 2.6) and the following two tables and graphical representations illustrate the outputs for both non-Article 5 and Article 5 using those assumptions:

Table 4-2: Non-Article 5 countries - HFO emissions (MIT-5 to 2050)

					HFO Annual Emissions (tonnes)			
Scenario	**Sector**	**Equipment Life (years)**	**HFO Allocation (%)**	**Emissions Rate/year (%)**	**2025**	**2050**	**2075**	**2100**
Plateau after 2050	Commercial	30	50	15	3,129	15,336	16,211	16,526
	Industrial	30	20	10	1,909	4,329	6,912	7,003
	Transport	15	50	30	421	1,256	1,375	1,375
	Stationary A/C	30	50	25	32,963	149,354	140,699	142,656
	Mobile A/C	15	50	35	16,502	58,365	67,025	67,025
	Total				**54,923**	**228,641**	**232,222**	**234,585**
Phase-out after 2050	Commercial	30	50	15	3,129	15,336	2,884	0
	Industrial	30	20	10	1,909	4,329	1,265	0
	Transport	15	50	30	421	1,256	0	0
	Stationary A/C	30	50	25	32,963	149,354	25,653	0
	Mobile A/C	15	50	35	16,502	58,365	0	0
	Total				**54,923**	**228,641**	**29,802**	**0**

Graphical representations of the data in the table above are provided in the following figure:

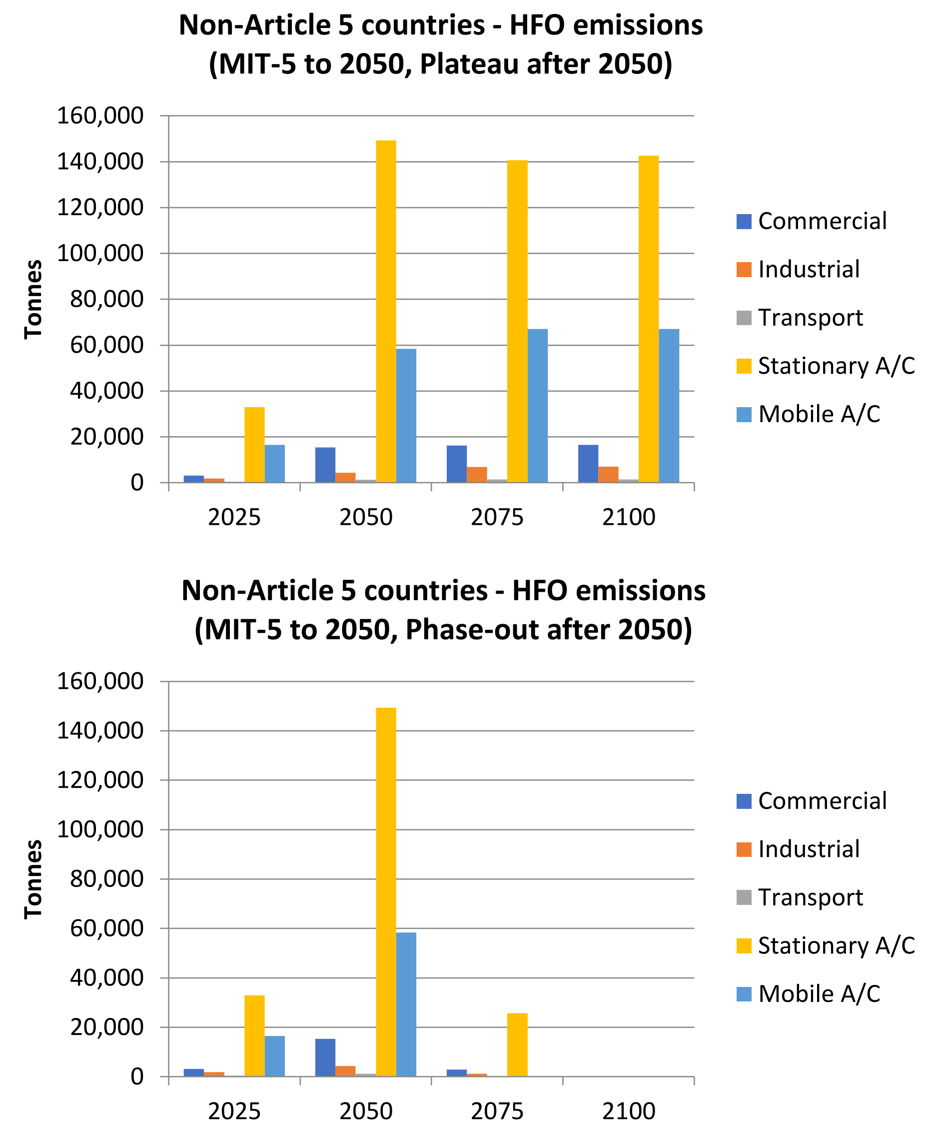


Figure 4-2: Non-Article 5 countries- HFO emissions (MIT-5), plateau (top graph) and phase-out (bottom graph) after 2050

Table 4-3: Article 5 countries - HFO emissions (MIT-5)								
					HFO Annual Emissions (tonnes)			
Scenario	Sector	Equipment Life (years)	HFO Allocation (%)	Emissions Rate/year (%)	2025	2050	2075	2100
Plateau	Commercial	30	50	20	2,085	169,169	237,429	238,511
	Industrial	30	20	15	5,833	20,223	32,197	32,398
	Transport	15	50	30	92	4,287	6,412	6,412
	Stationary A/C	30	50	30	13,491	564,598	411,646	400,868
	Mobile A/C	15	50	40	3,227	120,305	189,288	189,288
	Total				**24,728**	**860,582**	**876,971**	**867,477**
Phase-out	Commercial	30	50	20	2,085	169,169	45,081	0
	Industrial	30	20	15	5,833	20,223	6,070	0
	Transport	15	50	35	92	4,287	0	0
	Stationary A/C	30	50	30	13,491	546,598	88,365	0
	Mobile A/C	15	50	40	3,227	120,305	0	0
	Total				**24,728**	**860,582**	**139,516**	**0**

Graphical representations of the data in the table above are provided in the following figure:

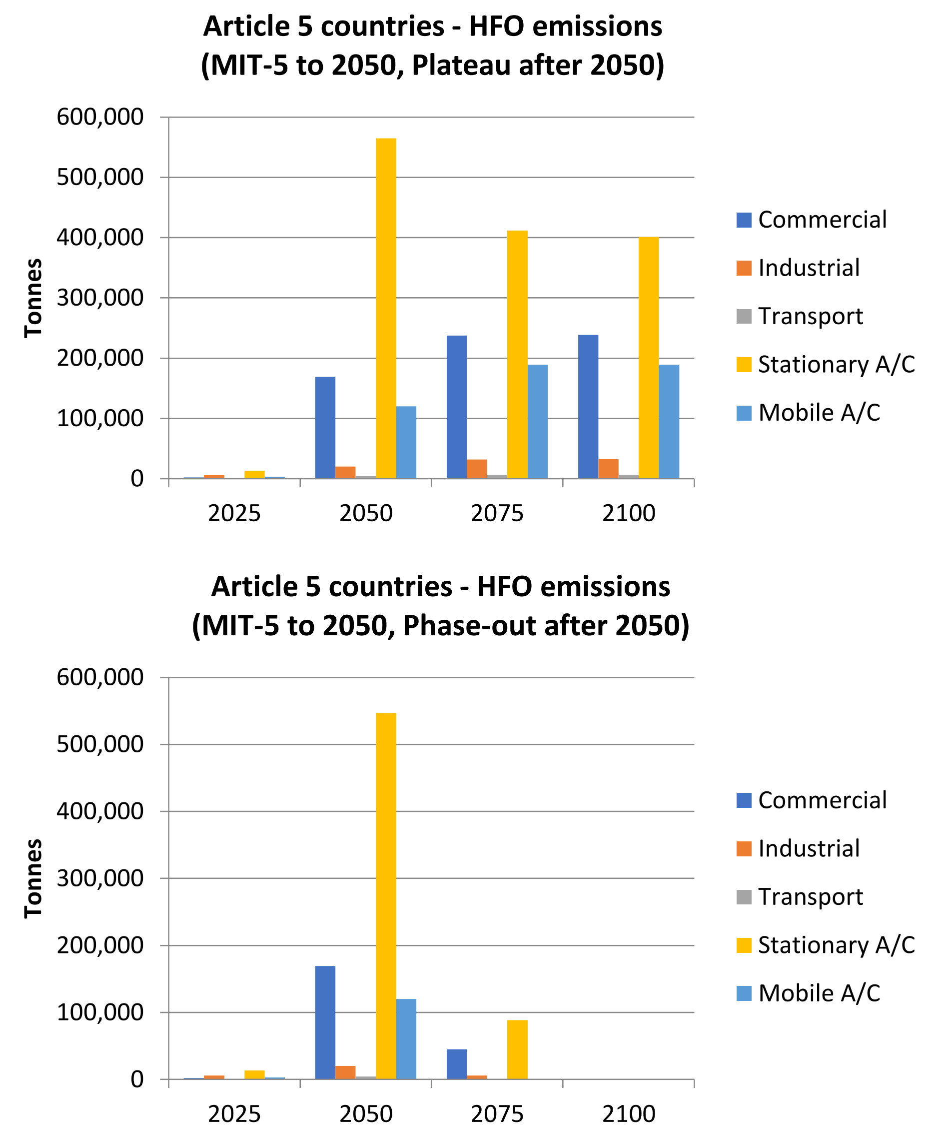


Figure 4-3: Article 5 countries - HFO emissions (MIT-5), plateau (top graph) and phase-out (bottom graph) after 2050

It can be seen by comparing these two tables that default emission factors have been considered to be 5% higher for Article 5 countries, reflecting the fact that best practice usually permeates from the non-A5 countries with something of a time-lag. Again, this is seen to promote a relatively conservative risk assessment in the final analysis.

4.2.3 Discussion/comparison of the results from BAU and MIT-5 scenario up to 2050

When comparing the BAU and MIT-5 outputs for the non-A5 contribution, it can be seen that the major impact of the mitigation scenario is in the Stationary A/C sector, where emissions of low-GWP refrigerants, including HFOs, are seen to climb steeply in the period to 2050. When adding the A5 contribution, the emissions could get to exceed 500,000 tonnes per year at their peak reflecting the likely dominance of demand and consumption in what are now developing regions as their economies mature and population factors become the key drivers. The distribution of these emissions is far from certain and may need closer monitoring over the coming years as the trends of the 21st century unfold.

While the modelled numbers are stated as they are calculated (i.e. to six significant figures in some cases), this should not be seen as a proxy for accuracy. The model has a number of approximations and assumptions that need to be understood, one of which is the fact that the annual consumption figures are linearly extrapolated between the five yearly data points provided by TEAP. Despite these limitations, it is believed that this approach offers a sufficiently robust input to give confidence on the outputs of any risk assessment conducted at global or regional level. The model would clearly not offer much value in local assessments, where specific factors are likely to dominate.

4.3 The impact of 'natural' refrigerants on HFO consumption

When considering the future size of the market for HFO refrigerants in both domestic and commercial implications, alternative refrigerant technologies need to be considered. The growth of alternative refrigerant technologies will have a bearing on the predicted HFO consumption and emissions from HFO-based technologies.

Natural refrigerants, mainly carbon dioxide (CO_2) (R-744) and hydrocarbons (R-290 (propane), R-1270 (propylene), and R-600a (isobutane)) are witnessing a high rate of adoption by major superstore and food retail chains in the European and North American regions.

The GWP of CO_2 is 1, however, the challenge for CO_2 is the high pressure needed for operation. Therefore, engineering standards need to be high but this can be bypassed by using secondary circuit systems in refrigeration. Hydrocarbons have a flammability issue and have a non-zero GWP but are still very low compared to HFCs. Ammonia (R-717) is also a potential natural refrigerant with a GWP of zero. However, there are toxicity issues associated with ammonia.

The number of CO_2-based stores in the EU, Norway and Switzerland has tripled in the last 3 years and now has 8% of the overall market share in the food retail market (see figure overleaf). Despite earlier claims that there are no viable solutions for warmer climates, the number of new installations is growing steeply in southern Europe also.

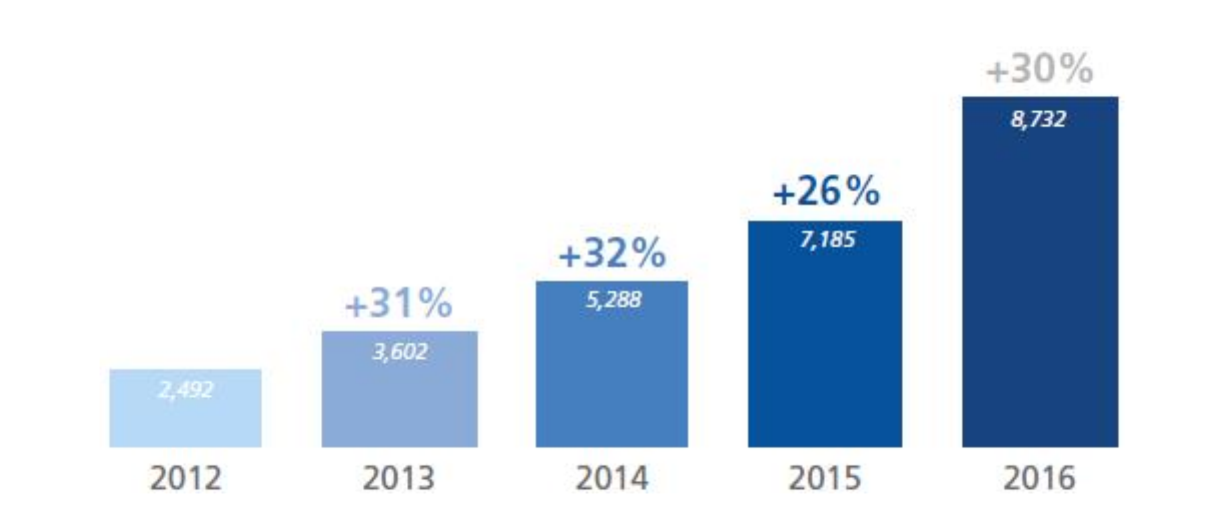


Figure 4-1: Growth of CO_2-based stores in the EU, Norway and Switzerland (estimate value for 2016)
Source: Jan Dusek, Shecco. Available at:
http://www.atmo.org/presentations/files/5907fb91732731493695377MIjnG.pdf

5 Chemical processes and degradation products

5.1 Chemical processes

The carbon double bond in HFOs (for example, see Figure 3-1,3-2 and 3-3) results in the reaction with atmospheric hydroxyl radicals being two orders of magnitude faster than with HFC-134a, which has a carbon to carbon single bond. This results in very short atmospheric lifetimes of a few days, which means that these compounds have negligible GWPs. For example, the atmospheric lifetime of HFO-1234yf is estimated to be approximately 6 days (Luecken et al, 2010) compared to HFC-134a with a lifetime of 14 years (Solomon et al, 2016 and references therein). Moreover, as they contain no bromine or chlorine atoms and are destroyed in the lower atmosphere, they do not contribute to stratospheric ozone depletion as seen with CFCs (Hansen et al, 2015). The atmospheric degradation of HFOs is discussed below.

5.1.1 Atmospheric dispersion and degradation mechanisms

The atmospheric dispersion of HFOs has been discussed extensively in the literature, with the primary focus on HFO-1234yf. In the atmosphere, there are two decomposition pathways that HFO-1234yf undergoes (Luecken et al, 2012; Russell et al, 2012):

Pathway 1, reaction with hydroxyl radicals ($^{\cdot}OH$), produces a 100% yield of trifluoroacetyl fluoride (CF_3COF, TFF) whilst reaction with chlorine radicals (equation 2) produces a 92% yield of TFF.

$$CH_2{=}CFCF_3 + {}^{\cdot}OH \rightarrow CF_3COF + HCHO + H_2O + XO_2 \quad (1)$$

$$CH_2{=}CFCF_3 + Cl^{\cdot} \rightarrow 0.92CF_3COF + 0.568{*}HC(O)Cl + 2XO_2 + CO \quad (2)$$

There are also reactions with ozone (O_3) and nitrate radical (NO_3) although these are considered to be of minor importance (Henne et al, 2012b).

The products (intermediates) of pathway (1) are TFF and formaldehyde (HCHO) and pathway (2) TFF and formyl chloride (HC(O)Cl). TFF then reacts rapidly with atmospheric moisture (H_2O) to form trifluoroacetic acid (CF_3COOH, TFA):

$$CF_3COF + H_2O \rightarrow CF_3COOH + CO_2 + HF \quad (3)$$

The dominant degradation pathway of HFO-1234yf is via reaction with hydroxyl radicals with a detailed pathway presented below in Figure 5-1. The first step in the process is addition of $^{\cdot}OH$ to one or other of the carbon atoms attached to the double bond, this is the rate-determining step. This is followed by a series of oxidation reactions involving molecular oxygen and nitric oxide (NO) resulting in the intermediates TFF and HCHO given in equation (1) above.

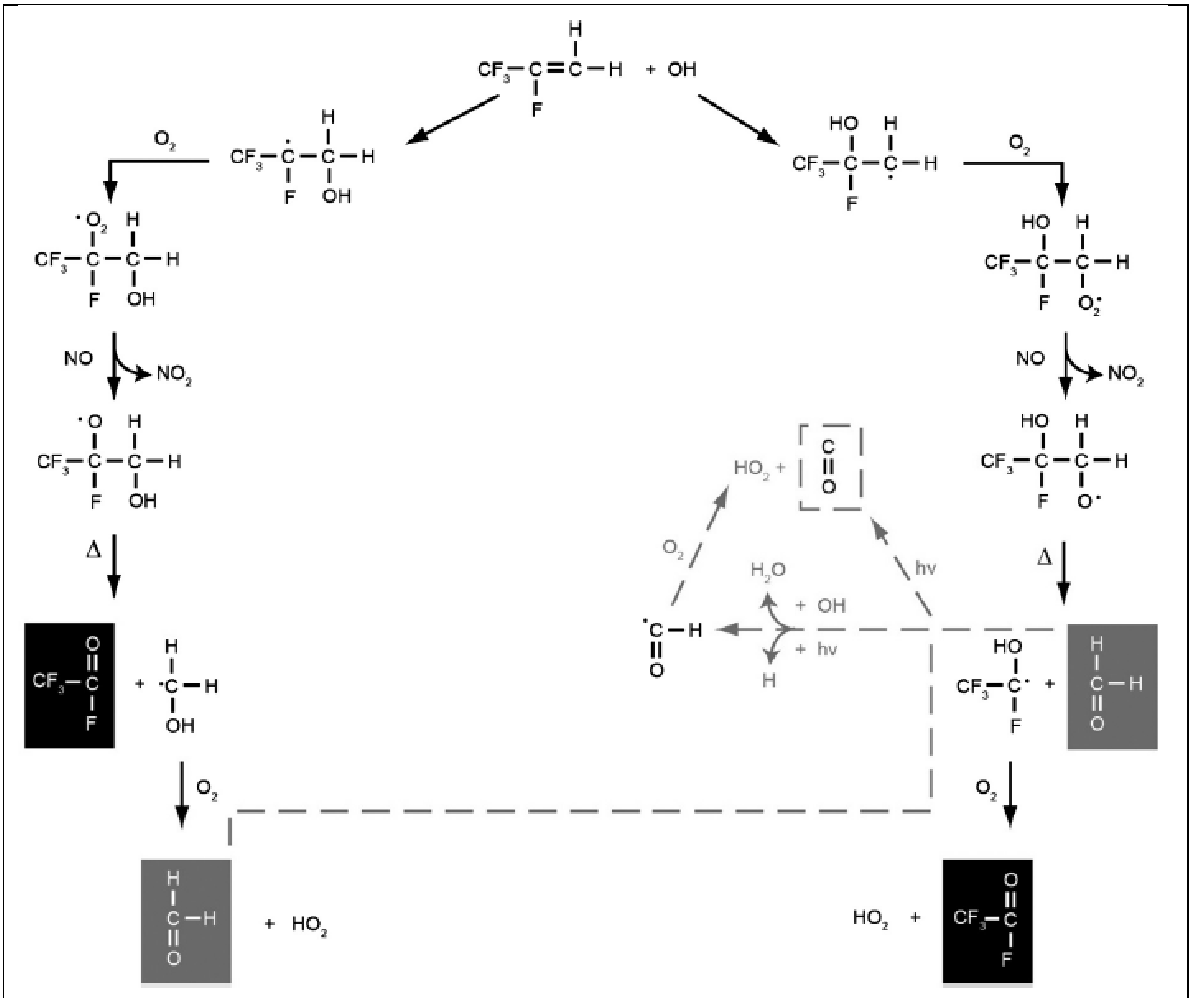


Figure 5-1: Atmospheric degradation mechanism for HFO-1234yf
Source: Wallington et al (2014): Atmospheric chemistry of sort-chain haloolefins: Photochemical ozone creation potentials (POCPs), global warming potentials (GWPs), and ozone depletion products (ODPs). Chemosphere, 129, pp 135-141

The potential for formation of photochemical ozone at ground level is low for these compounds since they have fewer or no carbon-hydrogen bonds than their alkyl equivalents and react slowly with atmospheric radicals. Papasavva et al discuss that HFO-1234yf also has the potential to form ozone in the troposphere with a maximum averaged incremental reactivity of 0.267 g ozone/g VOC for the overall atmospheric reactivity of the HFO (Papasavva et al, 2009). No photolysis of HFOs is also expected in the troposphere (Gonzalez et al, 2016).

5.2 Degradation products

Intermediate degradation products are dependent of the type of HFO and include, $CF_3C(O)F$ (TFF), HCHO (formaldehyde), $CF_3C(O)H$ (trifluoroacetaldehyde) and HC(O)F (formyl fluoride) (Table 5-1) (Hansen et al, 2015; Henne et al, 2012b).

For HFO-1234ze(E), the thermally unstable intermediates trifluoroacetaldehyde, $CF_3C(O)H$ and formyl fluoride, HC(O)F do not exist for long in the environment with $CF_3C(O)H$ photolysed by sunlight in the lower atmosphere, giving it a lifetime of 4 days. It is removed four times as fast as it is formed from HFO-1234ze(E) so cannot accumulate in the atmosphere. Formyl fluoride dissolves in environmental water where it is rapidly hydrolysed to hydrofluoric acid, HF and formic acid, HC(O)OH.

Table 5-1: Decomposition products of HFOs		
HFO substance	**Intermediate products**	**Final products**
HFO-1234yf	$CF_3C(O)F$ (trifluoroacetyl fluoride, TFF), HCHO (formaldehyde)	$CF_3C(O)OH$ (trifluoroacetic acid, TFA), CO_2 (carbon dioxide), HF (hydrofluoric acid)
HFO-1234ze(E)	$CF_3C(O)H$ (trifluoroacetaldehyde), HC(O)F (formyl fluoride)	CO_2, HC(O)OH (formic acid), HF
HFO-1216	$CF_3C(O)F$, COF_2 (carbonyl fluoride)	$CF_3C(O)OH$, CO_2, HF
HFO-1233zd(E)	$CF_3C(O)F$, HC(O)Cl, HCl (hydrochloric acid), $CF_3CH{=}CHOH$	CO_2, HF, HCl
HFO-1233zd(Z)	$CF_3C(O)F$, HC(O)Cl, HCl, $CF_3CH{=}CHOH$	CO_2, HF, HCl
Source: Wallington et al (2014): Atmospheric chemistry of sort-chain haloolefins: Photochemical ozone creation potentials (POCPs), global warming potentials (GWPs), and ozone depletion products (ODPs). Chemosphere, 129, pp 135-141		

Many studies such as those by Henne et al and Luecken et al, focus on TFA, see section below for further detail, when discussing degradation products of HFOs, namely HFO-1234yf, with only a minor consideration of other decomposition products such as HF and formic acid (Henne et al, 2012a; Luecken et al, 2010). HF and formic acid have large natural sources, for example, volcanic activity is a source of HF to atmosphere (Henne et al, 2012a). While HF might be a hazardous air pollutant, it is highly soluble and rapidly dissolved in rainwater and will add very little to total fluoride flux in the environment. HF is a strong acid, however, as highlighted from consultation with an academic expert, the buffering capacity of surface waters means HF is rapidly neutralised. Consequently, the amount of HF produced from current and expected future concentrations of HFCs and HFOs is also insignificant with respect to acidification (Hansen et al, 2015). There is also the potential that both monofluoroacetic acid and difluoroacetic acid may be produced from the degradation of HF (World Metrological Organisation, 2010). Formic acid is ubiquitous in the gaseous atmosphere and, due to its solubility in water, is widely distributed in rain and cloud water (Chebbi and Carlier, 1996). The final product CO_2 is a persistent greenhouse gas, however the contribution from this source is negligible compared with the total CO_2 burden.

The final degradation products are dependent on the identity of the HFO (Table 4-1), with TFA the main decomposition product for HFO-1234yf and HFO-1216, discussed in further detail in the section below (Wallington et al, 2014; Vollmer et al, 2015). Information from consultation indicates that HFO blends may not result in different products compared to those of pure HFOs and HFCs, as they will be single molecule reactions in the stratosphere. Incidentally, the breakdown of HFO-1234yf also results in the same decomposition products of the HFC it is replacing, HFC-134a (Minor et al, 2008).

5.2.1 TFA

A potential toxic by-product of the atmospheric degradation of HFOs is TFA which forms the main degradation product of some HFOs, as mentioned in the above section (Hansen et al, 2015). Gaseous TFA is rapidly partitioned into water droplets in the atmosphere and deposited on land and surface waters via wet precipitation (rain, snow and fog). Due to TFA being a strong acid, it readily forms trifluoroacetate salts (CF_3COO^-) with minerals in soil and surface waters.[2] This results in accumulation

[2] The stable form of TFA in the environment is the trifluoroacetate ion (CF_3COO^-) which will be combined with ions such as sodium and calcium to form neutral salts. However, TFA is readily used as an abbreviation for trifluoroacetic acid and its salts.

in playas, salt lakes and oceans where it combines with cations such as calcium, sodium and potassium (UNEP Ozone Secretariat, 2015). It is generally regarded as environmentally stable in aerobic soil and surface water though it may be co-metabolically degradable under anaerobic conditions (Russell et al, 2012).

There are a number of anthropogenic and natural sources of TFA and TFA salts in the environment. It's a degradation product of several of the HCFCs, HFCs (Boutonnet et al, 1999) and HFOs, with the yield dependent on the identity of the compound. TFA is also widely used in the chemical industry with the amounts being released to the environment highly uncertain; perfluorinated compounds and pharmaceutical products also contribute to TFA in the environment.

HFO-1234yf conversion to TFA is 1:1 on a molar and w/v basis, 100% molar yield, (Solomon et al, 2016 and references therein) which is a significantly higher yield than that of HFC-134a (Table 5-2) (Luecken et al, 2010).

Table 5-2: Molar yields of TFA from the degradation of HFOs and HFCs

Compound	TFA molar yield (%)
HFOs	
trans-HFO-1234ze*	<10% (as cited by WMO, 2010) (Note: Wallington et al, 2014 states TFA not formed)
HFO-1234yf*	100% (as cited by WMO, 2010; Solomon et al, 2016 and references therein)
HFCs	
HFC-134a	21% (as cited by Luecken et al, 2010)
HFC-227ea	100% (as cited by WMO, 2010)
HFC-245fa	<10% (as cited by WMO, 2010)
HFC-365mfc	<10% (as cited by WMO, 2010)
HFC-236fa	<10% (as cited by WMO, 2010)

Sources: Luecken et al (2010): Ozone and TFA impacts in North America from degradation of 2,3,3,3-Tetrafluoropropene (HFO-1234yf), a potential greenhouse gas replacement. Environ. Sci. Technol., 44, pp 343–348
World Meteorological Organisation (2010): Global Ozone Research and Monitoring Project—Report No. 52. Scientific Assessment of Ozone Depletion: 2010. World Meteorological Organization, National Oceanic and Atmospheric Administration, National Aeronautics and Space Administration, United Nations Environment Programme and the European Commission. Available at: https://www.wmo.int/pages/prog/arep/gaw/ozone_2010/documents/Ozone-Assessment-2010-complete.pdf
Solomon et al (2016): Sources, fates, toxicity, and risks of trifluoroacetic acid and its salts: Relevance to substances regulated under the Montreal and Kyoto Protocols. Journal of Toxicology and Environmental Health Part B., 19, pp 289-304
(*Referenced as trans-HFC-1234ze and HFC-1234yf in WMO,2010 report)

The 2005 IPCC/TEAP assessment estimated that HFC-134a decomposition was responsible for the production of 4,560 tonnes of TFA per year (IPCC/TEAP, 2005). The replacement of the current HFCs by HFO is likely to increase TFA concentrations due to the higher TFA molar yields compared with HFC.

6 Environmental impacts

6.1 Environmental compartments where TFA is found

TFA is found in a large number of environmental compartments summarised in the table below. Residues of TFA have been observed in water and air samples from many locations (USA, Canada, Australia, South Africa, Germany, Israel, Ireland, France, Switzerland, Finland, and China) and show that TFA is a ubiquitous contaminant of the hydrosphere (Solomon, 2003).

Table 6-1: Environmental compartments where TFA is found

Environmental compartment	Inflow and outflow
Air	Formed in the air but rapidly partitioned to water droplets
Clouds, rain, fog	Partitioning from air into water droplets
Soil	Inflow from dry or wet precipitation. Outflow via runoff, soil water and groundwater
Oceans, salt lakes, and playas	Inflow only, loss of water by evaporation only
Vernal pools	Small pools formed in shallow depressions from snowmelt and/or spring rains. Outflow to groundwater and/or loss by evaporation
Streams and rivers	Inflow from snowmelt, glaciers, rain, runoff from land, groundwater (springs), and water-treatment facilities. Outflow to oceans, salt lakes, or playas
Wetlands	Inflow from snowmelt, glaciers, rain, runoff from land, groundwater (springs), and water-treatment facilities. Outflow to streams and rivers
Source: Solomon et al (2016): Sources, fates, toxicity, and risks of trifluoroacetic acid and its salts: Relevance to substances regulated under the Montreal and Kyoto Protocols. Journal of Toxicology and Environmental Health Part B., 19, pp 289-304	

6.1.1 TFA in surface waters

In the atmosphere, a rapid partitioning of TFA into droplets of clouds, rain and fog occurs (Solomon et al, 2016). Wet precipitation (rain, snow and fog) is assumed to be the major source of TFA in the biosphere, e. g. for Switzerland, it was calculated that wet deposition accounts for 96% of the annual mass flux (Berg et al, 2000). TFA is found in rivers, streams, lakes and wetlands where inflow into these water bodies occur from precipitation, glaciers, runoff from land, groundwater (springs) and water-treatment facilities (Section 6.2.1 provides further details of concentrations found in rainwater and snow, and surface waters in the environment). About one third of the overall TFA is dislocated by rivers, which results in a considerable amount introduced in terrestrial environments where TFA is susceptible to leaching into the groundwater (Scheurer et al, 2017). A study indicated the TFA was infrequently detected in groundwater and the concentrations were low, ≥23 ng/L (Nielsen et al, 2001). This is unexpected as TFA is poorly retained in soil and has large mobility but may be due to the slow percolation into the groundwater samples that have been tested to date. Groundwater samples collected in Beijing also had a low TFA concentration of 10 ng/L (Zhang et al, 2005).

Hydrothermal vents are suggested as one of the natural sources of TFA in the oceans with data indicating that a large amount of the TFA salts in the ocean are from natural rather than anthropogenic sources (Solomon et al, 2016). It has been suggested that more than 95% of the TFA salts found in the oceans are naturally produced (UNEP EEAP, 2014). Evidence suggests that TFA can be 'evaporated' from ocean surfaces into the atmosphere which includes mechanical transport as aerosol and also vapourisation (EFCTC, 2016), although this is not indicated in Figure 6-1 of the water cycle below. Subsequently, it is removed from the atmosphere via wet precipitation and deposited to oceans and land; dry deposition of TFA to land also occurs as stated in Table 6-1 above.

TFA in freshwaters is thought to be anthropogenic in nature with natural occurrence controversially discussed. For example, TFA was not found in samples from older German and Swiss groundwater (Jordan and Frank, 1999; Berg et al, 2000). In another study, five samples of pre-industrial (>2000 year old) freshwater from Greenland and Denmark were collected; there was no detectable TFA (<2 ng/L) present in any of these samples (Nielsen et al, 2001). TFA in the atmosphere and precipitation is thought to be largely anthropogenic in nature with a study by Henne et al concluding that major present day contributions of TFA in the atmosphere, precipitation and surface fresh waters is anthropogenic, originating from the atmospheric oxidation of HFCs (Henne et al, 2012b).

It has been postulated that high concentrations of TFA in rain positively correlate with the degree of urbanisation/industrialisation in the catchment area (Scott et al, 2005b; Wang et al, 2014). However, Berg et al found no difference between precipitation samples collected in a densely populated catchment close to the city of Zurich and those of a remote alpine sampling site (Berg et al, 2000).

6.1.2 TFA in soils

TFA is deposited to land (soil) via wet precipitation (wet deposition) and also dry precipitation (dry deposition) of TFA from the atmosphere to the land. Dry deposition appears to be minor in comparison with wet deposition with Berg et al calculating that wet deposition accounted for 96% of the annual mass flux of TFA in Switzerland (Berg et al, 2000).

TFA forms salts with minerals in soil and although TFA is generally regarded as environmentally stable in aerobic soil (Russell et al, 2012), retention is poor. However, soils with high levels of organic matter have been shown to have a greater affinity for TFA when contrasted to soils with low levels of organic matter. This appears to be an adsorption phenomenon, not irreversible binding. Therefore, TFA will not be retained in soil, but will enter the aqueous environment such as rivers via surface runoff, groundwater and ultimately terminal sinks such as oceans and salt lakes (Boutonnet et al, 1999). Section 6.2.1 provides further details of concentrations of TFA found in soils in the environment.

6.1.3 Terminal sinks and hotspots

As seen in the figure below, TFA accumulates in playas, salt lakes and oceans (terminal sinks) where it combines with cations such as calcium, sodium and potassium (UNEP Ozone Secretariat, 2015). In these terminal sinks, inflow of water from rivers and streams occurs but no outflow is possible with loss of water by evaporation only (UNEP EEAP, 2015; Solomon et al, 2016).

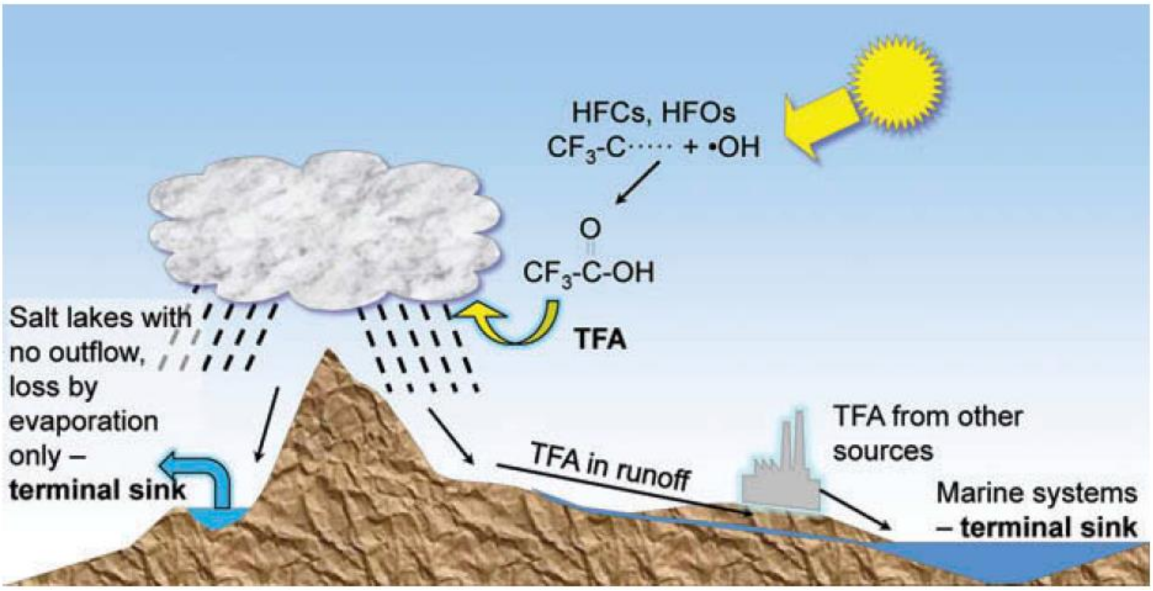


Figure 6-1: The fates of TFA and its salts in the environment
Source: Solomon et al (2016): Sources, fates, toxicity, and risks of trifluoroacetic acid and its salts: Relevance to substances regulated under the Montreal and Kyoto Protocols. Journal of Toxicology and Environmental Health Part B., 19, pp 289-304

A value of 200 ng a.e./L[3] for the concentration of TFA salts is considered to be representative in the oceans. The estimated contribution from continued use of HCFCs, HFCs, and HFOs up to 2050 was estimated to be a small fraction, 15.3 ng a.e./L, (<7.5%) of TFA present at the start of the millennium (UNEP EEAP, 2015). Some terminal sinks such as the Dead Sea have a concentration of 6,400 ng a.e./L with the large concentration here attributed to the collection of TFA salt over thousands of years, before significant anthropogenic affects (Boutonnet et al, 1999). More detailed analysis of concentrations of TFA in water bodies globally and the environmental effects of this substance are presented in Section 6.2.

Modelling studies have been conducted to determine the effects on TFA emissions if HFO-1234yf was used in mobile air conditioning. One study which considered the replacement of HFO-1234yf with HFC-134a as a cooling agent in mobile air conditioners predicted that about 30–40% of the European HFO-1234yf emissions would be deposited as TFA within Europe, while the remaining fraction was exported toward the Atlantic Ocean, Central Asia, Northern, and Tropical Africa. The largest annual mean TFA concentrations in rainwater were simulated over the Mediterranean and Northern Africa, with values up to 2500 ng/L, with maxima over the continent of about 2000 ng/L which occurred in the Czech Republic and Southern Germany (Henne, 2012b). Another similar study modelled the potential concentrations of TFA in terminal water bodies over extended periods if HFO-1234yf was used in mobile air conditioners. After 50 years of continuous emissions, aquatic concentrations of 1,000-15,000 ng/L were predicted, with extremes of up to 50,000-200,000 ng/L in settings such as the Sonoran Desert along the California/Arizona (USA) border (Russell et al, 2012).

Although TFA is a persistent toxic pollutant, it was estimated that if HFO-1234yf were used in place of all HFC-134a that is currently in use, predicted concentrations of TFA in terminal water bodies is not

[3] It is this salt form of TFA that is relevant to exposures in the environment. Where concentrations of salts were measured as TFA acid, the abbreviation a.e. (acid equivalents) is used.

expected to harm aquatic systems significantly, even considering potential emissions over extended periods. While the environmental effects of TFA are considered to be negligible over the next few decades, potential longer-term impacts could require future assessments due to the environmental persistence of TFA and uncertainty in future uses of HFOs (Huret et al, 2014). A common consensus is that more research is needed to fully understand the cycle of TFA in the atmosphere and hydrosphere and this has been highlighted as a gap in knowledge at present (Calm et al, 2012).

6.2 Environmental effects of TFA

The concentrations of TFA found in the environment are discussed below. They vary with the identity of the environmental compartment and the location, with the highest concentrations witnessed in terminal water bodies.

6.2.1 Concentrations of TFA in the environment

Rainwater and snow

TFA concentrations in rainwater can be highly variable from one location to another. Measurements in rain and snow in Switzerland have shown TFA levels from 3-1550 ng a.e./L (Berg et al, 2000). In a study in Chile, Malawi, and Canada, ranges of concentrations of TFA in rainwater were 6-87, 4-15, and <0.5-350 ng a.e./L, respectively (Scott et al, 2005). TFA concentrations were measured in rainwater in two cities in Japan with values in the range 29-76 ng a.e./L (Taniyasu et al, 2008). In Guangzhou, China (located in the Pearl River delta), concentrations of TFA in rainwater measured during April 2007-March 2008 ranged from 46-974 ng a.e./L (Wang et al, 2014).

Soils

In terrestrial systems, the first points of contact of precipitation (rain, fog and snow) are vegetation, soil, and surface water. Once in contact with soil or surface water, TFA reacts with minerals to form salts. Although TFA is generally regarded as environmentally stable in aerobic soil, retention is poor (Russell et al, 2012). TFA will not be retained in soil and will enter the aqueous environment and ultimately terminal water bodies (Boutonnet et al, 1999). The concentrations measured in soil are relatively small with values in the range <0.0-1,400 ng a.e./kg dry weight (d.w.) of soil in Canada, in Malawi, <100-7,500 ng a.e./kg d.w.; in the UK, 850-5,000 ng a.e./kg d.w.; and in Chile 100–9,400 ng a.e./kg d.w. (Solomon et al, 2016 and references therein).

Surface waters

As seen in the table below, concentrations of TFA measured in surface waters vary widely with location and type of water body.

Table 6-2: Concentrations of TFA in surface fresh waters		
Location and type of water body	**Range of concentrations in ng a.e./L**	**Reference**
Northern California		
Surface water	5-300	Cahill and Seiber (2000): Regional distribution of trifluoroacetate in surface waters downwind of urban areas in Northern California, U.S.A. Environmental Science & Technology, 34, pp 2909–12; Cahill et al (2001): Accumulation of trifluoroacetate in seasonal wetlands in California. Environmental Science & Technology, 35, pp 820–25
Yukon and Alaska		
Surface waters	8-27	Cahill and Seiber (2000)
British Columbia		
Surface waters	21-63	Cahill and Seiber (2000)
Germany		
Rivers	5,400-140,000	Scheurer et al (2017): Small, mobile, persistent: Trifluoroacetate in the water cycle - Overlooked sources, pathways, and consequences for drinking water supply. Water Research, 126, pp 460-471
Switzerland		
Rivers	12-328	Berg et al (2000): Concentrations and mass fluxes of chloroacetic acids and trifluoroacetic acid in rain and natural waters in Switzerland. Environmental Science & Technology, 34, pp 2675–83
Midland lakes	37-204	
Mountain lakes	46-360	
Moor water	59-175	
Drinking water	16-123	
Beijing		
Surface waters	380-820	Zhai et al (2015): A 17-fold increase of trifluoroacetic acid in landscape waters of Beijing, China during the last decade. Chemosphere, 129, pp 110–17. Samples taken in 2012; values had increased by 17-fold since previous analyses in 2002 by Zeng et al. (2004): Determination of trifluoroacetic acid in surface water of Beijing. Researcher Environment Sciences, 17, pp 64–67
Drinking water	155	

The Dead Sea (a salt lake) has a concentration of 6,400 ng a.e./L with the large concentration here attributed to the collection of TFA salt over thousands of years, before significant anthropogenic affects (Boutonnet et al, 1999). A modelling study predicted the potential concentrations of TFA in terminal water bodies over extended periods if HFO-1234yf was used in mobile air conditioners. After 50 years of continuous emissions, aquatic concentrations of 1-15 µg/L (1,000-15,000 ng/L) were predicted, with extremes of up to 50-200 µg/L (50,000-200,000 ng/L) in playas in the Sonoran Desert along the California/Arizona (USA) border (Russell et al, 2012).

Drinking water

Exposure of humans to TFA salts via drinking water was based upon the World Health Organization (WHO) default for consumption of 2 L water per day in a 60 kg human (World Health Organization 2008). The maximal concentration measured in drinking water and surface water was used as the exposure concentration and NOEC from the rat (Boutonnet et al, 1999) was used as the toxicity value. The margin of exposure (MoE) is calculated as 18,698,000 ng TFA salt/kg/day (normalised to the daily dose in a 60 kg person). The value is deemed sufficiently conservative to be protective for other vertebrates in the environment (Solomon et al, 2016).

Elevated concentrations of TFA of 5.4-140 µg/L were recently reported in Neckar River downstream of Bad Wimpfen, in South-west Germany. These elevated levels of TFA led concentrations of greater than 20 µg/L in bank filtration based tap waters. The source of the discharge was identified as a producer of inorganic and organic fluorinated chemicals. These values exceeded the German Federal Environment Agency specified health-related indication value (HRIV) of 1 µg/L (now 3 µg/L) for TFA in tap water. Upstream of the point of discharge the concentrations were much lower but TFA was still present with concentrations around 1 µg/L (Scheurer et al, 2017).

Oceans

The concentrations of TFA in the Mid-Atlantic and the Southern Ocean off Elephant Island were all close to 200 ng a.e./L at depths ranging from the surface to 4150 m. Those measured at various depths in the Western and Eastern Arctic, North Atlantic, and North and South Pacific were all ≤200 ng a.e./L and some were as low as 1 ng a.e./L. To conclude, a value of 200 ng a.e./L is considered to be a representative value for TFA concentrations in the oceans (Solomon et al, 2016 and references therein).

Acidification of freshwaters

A study by Wallington et al stated that the additional acidity in precipitation resulting from the atmospheric oxidation of HFOs will be negligible (Wallington et al, 2014) and no acidification of surface waters and terminal water bodies will be witnessed. There have been no reports suggesting that TFA lowers the pH of surface waters and consultation with an academic expert indicated that the buffering capacity of surface water means TFA is rapidly neutralised. The pK_a value of TFA is 0.23, making it a much weaker acid than sulphuric acid, H_2SO_4 (pK_a=-3) and will make negligible contribution to acid rain.

6.2.2 Toxicity of TFA

Playas and salt lakes (terminal sinks) contain more than the 35 g/L of salt found in the oceans. For example, the Great Salt Lake in Utah has concentrations of salts that vary from 50 to 270 g/L. These types of environments are only habitable to a small number of organisms that are highly tolerant of salts (halophiles) (Solomon et al, 2016). Furthermore, information gathered from consultation and literature indicates that other salts such as NaCl present in terminal sinks, namely playas and lakes, are much higher in concentration than those of TFA salts and predicted to be for the foreseeable future.

Regulatory activities

TFA classification, labelling and packaging

The table below summarises the self-classification, labelling and packaging (CLP) for trifluoroacetic acid and sodium trifluoroacetate. Twenty three classification and labelling notifications list sodium trifluoroacetate as Aquatic Acute 1 and Aquatic Chronic 1 whereas four notifications do not list aquatic toxicity.

Table 6-3: CLP classification of TFA		
Hazard Class and Category Code	**Hazard Statement Code**	
Trifluoroacetic acid (CAS No. 76-05-1; EC No. 200-929-3)		
Skin Corr. 1A	H314	Causes severe skin burns and eye damage
Acute Tox. 4	H332	Harmful if inhaled
Aquatic Chronic 3	H412	Harmful to aquatic life with long lasting effects
Sodium trifluoroacetate (CAS No. 2923-18-4; EC No. 220-879-6)		
Acute Tox. 2	H300	Fatal if swallowed
Aquatic Acute 1	H400	Very toxic to aquatic life
Aquatic Chronic 1	H410	Very toxic to aquatic life with long lasting effects
Sources: ECHA (2017): Trifluoroacetic acid Classification and Labelling. Available at: https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/47316 ECHA (2017): Sodium trifluoroacetate Classification and Labelling. Available at: https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/72268		

REACH registration dossier

However, ECHA (2017e) have requested that the lead registrant for TFA submit the requested information, summarised below, in an updated registration dossier by 7 January 2021, except for the information requested under point 1 for a sub-chronic toxicity study (90-day) which shall be submitted in an updated registration dossier by 9 July 2018.

1. *'Sub-chronic toxicity study (90-day), oral route (Annex IX, Section 8.6.2.; test method: EU B.26./OECD TG 408) in rats with the registered substance adjusted to physiological pH;'*

The study records provided by the registrant does not provide the information required by Annex IX, Section 8.6.2., because exposure duration is less than 90 days and not all tissues/organs are histopathologically investigated and not necessarily with the same statistical power as a study according to OECD TG 408 would require. Therefore, ECHA states that the information provided on this endpoint for the registered substance in the technical dossier does not meet the information requirement. Consequently, there is an information gap and it is necessary to provide information for this endpoint.

2. *'Pre-natal developmental toxicity study (Annex IX, Section 8.7.2.; test method: EU 8.3I./OECD TG 414) in a first species (rat or rabbit), oral route with the registered substance adjusted to physiological pH.'*

ECHA highlight that the registrant provided study records for three non-guideline studies, that there are methodological deficiencies in the studies and more specifically and these studies do not cover key parameters of pre-natal developmental toxicity effects *in vivo*. Therefore, ECHA state that the individual sources of information in the dossier do not provide the information required for this endpoint.

3. *Pre-natal developmental toxicity study (Annex X, Section 8.7.2.; test method: EU 8.3I./OECD TG 414) in a second species (rabbit or rat), oral route with the registered substance adjusted to physiological pH;'*

ECHA highlights that there is no information provided for a pre-natal developmental toxicity study in a second species. Therefore, the information provided on this endpoint for the registered substance in the technical dossier does not meet the information requirement. Consequently, there is an information gap and it is necessary to provide information for this endpoint.

4. *'Extended one-generation reproductive toxicity study (Annex X, Section 8.7.3.; test method: EU 8.56./OECD TG 443) in rats, oral route with the registered substance adjusted to physiological pH, specified as follows:*

   - Ten weeks premating exposure duration for the parental (PO) generation;
   - Dose level setting shall aim to induce some toxicity at the highest dose level;
   - Cohort 1A (Reproductive toxicity);
   - Cohort 1B (Reproductive toxicity) without extension to mate the Cohort 18 animals to produce the F2 generation.'

ECHA considers that there is not sufficient weight of evidence from several independent sources of information which would allow to assume/conclude that the substance does not have a particular dangerous property, i.e. reproductive toxicity. Therefore, ECHA concludes that the information provided on this endpoint for the registered substance in the technical dossier does not meet the information requirement. Consequently, there is an information gap and it is necessary to provide information for this endpoint.

5. *'Identification of PNEC and risk characterisation (Annex I, Section 3.3.1. and 6.): revise PNECs for freshwater, marine water, freshwater sediment and marine sediment using the study giving rise to the highest concern according to Annex I, Section 3.1.5 and revise the risk characterisation accordingly or provide a detailed justification for not using the recommendations of ECHA guidance in PNEC derivation.'*

ECHA highlights issues with the way PNEC values have been calculated and the lead registrant has been requested to revise PNECs for freshwater, marine water, freshwater sediment, marine sediment using the result giving rise to the highest concern, i.e. the NOEC of O.2 mg/L for *Raphidocelis subcapitata* (formerly known as *Selenastrum capricornutum* and *Pseudokirchneriella subcapitata*).

6. *'Exposure assessment and risk characterisation (Annex I, Sections 5. and 6.) for environment.*
   - Revise the exposure assessment to provide a detailed justification' including related risk management measures, for using non-default release factor in the exposure estimation for exposure scenarios ESl and ES2 or to apply default release factors according to ECHA Guidance R.16.
   - Revise the exposure assessment to apply a "fraction of the main source" of 100% for exposure scenarios ES3, ES4 and ES6 in accordance with the recommendations of ECHA Guidance R.16 or to provide adequate justification for any deviation from these recommendations.
   - The risk characterisation shall be revised accordingly.'

ECHA indicates that there is missing information on the risk management measures for manufacture of TFA on the plant (next words blocked out) and there are deviations on the assumed fraction used at main source (i.e. annual use amount at a site).

7. *'Exposure assessment (Annex I, Section 5.1.1.) for human health: provide documentation for the recommended personal protective equipment, i.e. hand and skin protection, respiratory protection and eye/face protection;*
   - specify the type of glove material, thickness and breakthrough times;
   - specify the filter type/class for the respiratory protective
   - specify the type and quality of protective clothing.'

ECHA highlights that specific detailed information on the recommended personal protective equipment (PPE) is missing both from the CSR and from the information on safe use within the IUCLID dossier. ECHA have requested the registrant provide more detailed information on the PPE above.

The updated REACH registration dossier for TFA will be available in 2021 and will address some of the toxicity data that is inadequate or absent which is highlighted in the sections below.

Mammal toxicity

TFA salts are neutral, chemically unreactive, and there is no known specific receptor to which TFA salts will bind to cause a biological response (Solomon et al, 2016). Potential for bioaccumulation of TFA and its salts in mammals is highly unlikely due to the extremely low Log K_{ow} (-0.2), it would be rapidly eliminated via the kidneys into the urine. There has been some evidence of incorporation of TFA into biomolecules with radiolabelled TFA being shown to bind covalently to proteins in blood of mammals (Boutonnet et al. 1999). However, TFA concentrations are not expected to rise in the food chain and trophic magnification would not occur as TFA is covalently bound to macromolecules and would be released during digestion and catabolism of these molecules (Solomon et al, 2016).

The acute oral NOEC (No Observed Effect Concentration) for TFA in rats is 250 mg a.e./kg body weight (b.w.) (Boutonnet et al. 1999). In mice, TFA exerted toxicity similar to that of hydrochloric acid. The acute NOEC for the sodium salt of TFA in rats is ≥5000 mg/kg b.w. The 8-d chronic oral NOEL (No Observed Effect Level) for the sodium salt of TFA in rats is 114 mg/kg b.w./d. For humans, the threshold for respiratory irritation after a 1 min exposure is 0.25 mg a.e./L of air. Furthermore, no carcinogenicity or reproductive toxicity tests on TFA or its salts have been published and bacterial assays for mutagenicity showed TFA salt was found to be inactive (Solomon et al, 2016).

Terrestrial toxicity

2-yr-old pine (*Pinus ponderosa*) seedlings were treated in fog chambers with TFA at concentrations of 150 and 10,000 ng a.e./L. They showed no adverse physiological, morphological, or photosynthetic responses (Benesch and Gustin 2002).

The effect of sodium trifluoroacetate (NaTFA) in soil on seed germination and early plant growth of sunflower (*Helianthus annuus*) and mung bean (*Phaseolus aureus*) was determined according to the testing OECD 208 guideline (ECHA, 2017d). The EC_{50}[4] for sunflower germination was 250 mg NaTFA/kg (208 mg TFA/kg) and for the mung bean was 770 mg NaTFA/kg. At the end of the test, 28 days after the seeds were sown, the mean fresh weight of the sunflower shoots was significantly reduced at all concentrations tested (at and above 1 mg/kg). Growth of mung bean was significantly reduced at and above 10 mg/kg. Consequently, the sunflower was assigned a NOEC of <1 mg NaTFA/kg and mung bean NOEC = 1 mg NaTFA/kg dry soil.

[4] The concentration that causes the measured effect in 50% of organisms.

Some bioaccumulation has been seen in higher plants such as sunflower and wheat. This was related to uptake with water and then concentration due to transpiration water loss (Tang et al, 1998 and references therein). Although uptake of TFA by plants has been shown, no measurements of the concentrations of TFA in crops for human consumption, both raw and processed foods, have been reported (Solomon et al. 2016).

From consultation with an academic expert, it was stated that even if rainwater with dissolved TFA lands on the surface of a leaf, it is unlikely to result in adverse effects for the plant. However, it has been noted in the literature that there is inadequate information on the toxicity of TFA and salts to terrestrial plants (Solomon et al, 2016). Therefore, doubts remain on whether increasing concentrations in ecosystems may have implications for terrestrial plants.

There appears to be no published data for toxicity to soil macroorganisms except arthropods, terrestrial arthropods and toxicity to birds or soil microorganisms. However, they would not be expected to be significantly more toxic to other vertebrates than to mammals (Solomon et al, 2016).

Aquatic toxicity

TFA is not concentrated in lower aquatic-life forms such as bacteria, small invertebrates, oligochaete worms, and some aquatic plants including *Lemna gibba* (duckweed). In acute toxicity tests no effects of NaTFA (sodium trifluoroacetate) on water fleas (*Daphnia magna*) and zebra fish (*Danio rerio*) were found at a concentration of 1200 mg/L (Berends et al, 1999).

A seven day study with duckweed (*Lemna gibba*) revealed an EC_{50} (frond increase) and EC_{50} (weight increase) of 915 and 999 mg/L of TFA, respectively. In a 35 day outdoor aquatic microcosm study with a mixture of TFA salt and trichloroacetic acid, no marked effects were observed in aquatic plants, *Myriophyllum spicatum* and *Myriophyllum sibiricum* (Hanson et al.2002).

Based on the results of five toxicity tests, *Raphidocelis subcapitata* (formally known as *Selenastrum capricornutum* and *Pseudokirchneriella subcapitata*) exhibited unique sensitivity with a NOEC of 0.12 mg/L (Tang et al, 1998; Russell et al, 2012). The current concentrations of TFA in natural surface waters are almost 1000 times inferior (Dalang, 2010). However, this organism needs retesting to confirm its sensitivity. Recovery of the growth of *Raphidocelis subcapitata* was found when TFA was removed from the test solutions; therefore TFA should be considered algistatic and not algicidal for this species; the reason for the unique sensitivity of this strain is unknown (Tang et al, 1998). Algal toxicity tests with NaTFA and *Chlorella vulgaris, Scenedesmus subspicatus*, *Chlamydomonas reinhardtii*, *Dunaliella tertiolecta*, *Euglena gracilis*, *Phaeodactylum tricornutum, Navicula pelliculosa*, *Skeletonema costatum*, *Anabaena flos-aquae* and *Microcystis aeruginosa* resulted in NOEC values which were all higher than 100 mg/L (Berends et al, 1999).

To determine toxicity to microorganisms, the influence of NaTFA on the activated sludge was evaluated. The respiration rate (oxygen consumption) of an aerobic activated sludge fed with a standard amount of synthetic sewage was measured in the presence of various concentrations of NaTFA (10, 32, 100, 320 and 1000 mg/L) after an incubation period of 3 hours. The inhibition of the bacterial respiration activity was in the range of 3.2 to 9.7% for the test concentrations of 10 to 1000 mg/L. The maximum inhibition was 9.7% at a test concentration of 100 mg/L. However, the 3 hour EC_{10}[5], EC_{20}[6] and EC_{50} could not be quantified (ECHA, 2017d).

There is no information in the literature on the potential toxicity effects of TFA on organisms found in salt lakes and playas. This is an issue as salt lakes are the most likely site for accumulation of TFA in the natural environment (Solomon et al, 2016).

A summary for aquatic toxicity for different species and their associated NOEC, EC_{10}, EC_{25}[7] and EC_{50} values are given in the table overleaf.

[5] The concentration that causes the measured effect in 10% of organisms

[6] The concentration that causes the measured effect in 20% of organisms

[7] The concentration that causes the measured effect in 25% of organisms

Table 6-4: Aquatic toxicity results for trifluoroacetic acid (TFAA) and sodium trifluoroacetate (NaTFA)						
Aquatic organism	Test chemical	NOEC (mg/L)	EC_{10} (mg/L)	EC_{25} (mg/L)	EC_{50} (mg/L)	Reference
Freshwater algae						
Raphidocelis subcapitata[a]	NaTFA	0.12	NA	NA	4.8	Berends et al (1999): Toxicity of trifluoroacetate to aquatic organisms. Environ. Toxicol. Chem., 18, pp 1053–1059
Euglena gracilis	NaTFA	112	NA	NA	>112	Ref. as previous
Microcystis aeruginosa	NaTFA	117	NA	NA	>117	Ref. as previous
Chlamydomonas reinhardtii	NaTFA	120	NA	NA	>120	Ref. as previous
Scenedesmus subspicatus	NaTFA	NA	NA	NA	>120	Ref. as previous
Navicula pelliculosa	NaTFA	600	NA	NA	1,200	Ref. as previous
Aphanizomenon flos-aquae	NaTFA	600	NA	NA	2,400	Ref. as previous
Chlorella vulgaris	NaTFA	1,200	NA	NA	>1,200	Ref. as previous
Marine algae						
Dunaliella tertiolecta	NaTFA	<124	NA	NA	>124	Ref. as previous
Phaeodactylum tricornutum	NaTFA	117	NA	NA	>117	Ref. as previous
Skeletonema costatum	NaTFA	2,400	NA	NA	>2,400	Ref. as previous
Aquatic plants						
Myriophyllum sibiricum[b]	TFAA	100	36.3	113.8	357.0	Hanson et al (2004): Haloacetic acids in the aquatic environment. Part I. Macrophyte toxicity. Environ. Pollut., 130, pp 371–383
M. spicatum[b]	TFAA	30	41.8	114.4	312.9	Ref. as previous
Lemna gibba[c]	TFAA	100	192.8	298.5	618.3	Ref. as previous
L. gibba	NaTFA	300	NA	NA	1,100	Berends et al (1999): Toxicity of trifluoroacetate to aquatic organisms. Environ. Toxicol. Chem., 18, pp 1053–1059
Crustacea						
Daphnia magna	NaTFA	1,200	NA	NA	>1,200	Ref. as previous
Fish						
Danio rerio	NaTFA	1,200	NA	NA	>1,200	Ref. as previous
[a]Formerly known as *Selenastrum capricornutum* and *Pseudokirchneriella subcapitata*; [b]Endpoint of wet mass; [c]Endpoint of frond increase TFAA=trifluoroacetic acid; TFA=trifluoroacetate; NA=not available						

The table below summarises the PNEC (Predicted No-Effect Concentration) values for organisms in different environmental compartments:

Table 6-5: Ecotoxicology summary for trifluoroacetic acid	
Hazard for aquatic organisms	**Hazard assessment conclusion**
Freshwater	PNEC aqua (freshwater) = 1 mg/L
Marine water	PNEC aqua (marine water) = 0.1 mg/L
STP[a]	PNEC STP = 83.2 mg/L
Sediment (freshwater)	PNEC sediment (freshwater) = 4.22 mg/kg sediment dw[b]
Sediment (marine water)	PNEC sediment (marine water) = 0.422 mg/kg sediment dw
Hazard for air	**Hazard assessment conclusion**
Hazard for air	No hazard identified
Hazard for terrestrial organisms	**Hazard assessment conclusion**
Soil	PNEC soil = 4.7 µg/kg soil dw
Hazard for predators	**Hazard assessment conclusion**
Secondary poisoning	No potential for bioaccumulation
Source: ECHA (2017): Trifluoroacetic acid registration dossier. Available at: https://echa.europa.eu/registration-dossier/-/registered-dossier/5203/6/1 [a]STP = Sewage treatment plant microorganisms; [b]dw = dry weight	

Summary of TFA toxicity

Of the tested aquatic organisms, only the alga *R. subcapitata* displayed sensitivity to TFA, although this needs to be confirmed by retesting. No published data for toxicity to soil macroorganisms except arthropods, terrestrial arthropods, toxicity to birds or soil microorganisms have been identified. There is less than satisfactory information on the toxicity of TFA and salts to terrestrial plants, and no studies have been reported for concentrations of TFA in crops for human consumption (Solomon et al. 2016). Furthermore, there is no information on toxicity to organisms found in salt lakes and playas. This is particularly important because salt lakes are the most likely site for accumulation of TFA in the natural environment. However, these types of environments are only habitable to a small number of organisms that are highly tolerant of salts (halophiles).

The estimated contribution of TFA to the oceans from the continued use of HCFCs, HFCs, and HFOs up to 2050 was estimated to be a small fraction, 15.3 ng a.e./L, (<7.5%) of TFA present at the start of the millennium (UNEP EEAP, 2015). It has also been suggested that the additional acidity in precipitation resulting from the atmospheric oxidation of HFOs will be negligible (Wallington et al, 2014). Evidence gathered from the literature review, and from consultation with two academic experts, suggests that current and estimated concentrations of TFA and its salts in the environment resulting from the degradation of HCFCs, HFCs and HFOs in the atmosphere do not present a risk to the environment. However, due to the persistent nature of TFA, concentrations continue to rise in terminal sinks. It has been suggested that increased monitoring of these terminal sink sites is required to develop a greater understanding of the effect increasing concentrations of TFA may have on the environment.

6.3 Environmental effects of other decomposition products

Information gathered from consultation with two academic experts, suggests that the formation of HF and formic acid from the atmospheric degradation of HFOs is not a significant issue for the environment and the same level of concern is not present as there is for TFA.

Hydrofluoric acid and hydrochloric acid

A major gap in knowledge identified during consultation was the lack of availability of data on the stoichiometry/quantity of HF produced from HFOs. However, HF is still not expected to have any effect on the environment.

Evidence from consultation with an academic expert indicated that HF is a strong acid, however, it is rapidly neutralised due to the buffering capacity of water to give fluoride salts in the environment. The additional acidity in precipitation resulting from the atmospheric oxidation of HFOs is expected to be negligible (Wallington et al, 2014). Therefore, no acidification of surface waters and terminal water bodies is expected.

HFOs/HCFOs will not be uniformly distributed in the atmosphere and hence the regional concentrations of HF/HCl will be greater than the global average by perhaps an order of magnitude (i.e., 10^{-8}-10^{-7} molar compared to global average of 10^{-9}-10^{-8}). The concentration of fluoride/chloride produced from the degradation of HFOs will have a negligible effect on the total fluoride/chloride flux in the environment.

Formic acid

The concentrations of formic acid produced from the degradation of HFOs are not known and information gathered about formic acid production was established from laboratory pathways. However, concentrations are expected to be low and will have no impact on organisms; formic acid is a naturally occurring intermediate in the body and ubiquitous in the natural environment (Wallington et al, 2014).

Carbonyl fluoride

Carbonyl fluoride is an intermediate formed during the degradation of some HFOs. Consultation with an academic expert, indicated that any intermediates produced from HFO degradation are very reactive (short-lived) and will not be present in high concentrations. Furthermore, a major manufacturer suggested during consultation that carbonyl fluoride produced from the degradation of HFOs is not an issue as the substance is extremely short-lived and rapidly hydrolysed to HF (Tsai, 2005).

7 Human health impacts

7.1 Hazards to human health

The effect of HFCs on human health has been studied and reported in the literature. Tsai (Tsai, 2005) reports that due to the physiochemical properties of HFCs there is low toxicity to human health. For example, for HFC-134a at an exposure level of 1000 ppm, there is NOAEL (No Observed Adverse Effect Level) and no LOAEL (Local Observed Adverse Effect Level). Exposure to HFCs is reported by Tsai to occur from the following activities:

- Leaks or spills from the refrigeration system;
- The electronic appliance recycling system; and
- Cleaning and gas delivery pipelines.

It is also worth noting that Tsai reports there is very limited information in the literature for human exposure to elevated HFC levels with only one study reporting moderate occupational exposure for short periods. It was noted that repair works involving welding could lead to exposure to decomposition products.

For HFOs, there is a lack of available literature on human health hazards from exposure. Broad range searches in PubMed resulted in no relevant studies, with Google Scholar also employed for identifying relevant studies. Human health hazards for HFOs are addressed in material safety data sheets and state they are asphyxiant in high concentrations and that contact with the evaporating liquid may lead to freezing of the skin or frostbite. Consultation has also confirmed that there is a lack of publically available information on the health effects of HFOs.

Under the ECHA CLP database, no health hazards have been identified for the HFO substances registered under REACH. For the HFO substances registered under REACH, human health hazards have been assessed and are summarised in the below table. From consultation, as part of the registration process with the United States Environmental Protection Agency (US EPA), companies are also required to inform the US EPA what workers are exposed to.

Table 7-1: Hazard information from HFOs used as refrigerants

HFO substance	Hazard to workers health
HFO-1234yf	Considered to be low hazard for inhalation exposure, dermal exposure and eyes. No thresholds for the hazard have been identified
HFO-1234ze	No hazard has been identified for inhalation. The hazard is unknown for dermal and eye exposure
HFO-1233zd	No hazard has been identified for inhalation, dermal and eye exposure

Sources: ECHA (2017): Polyhaloalkene registration dossier. Available at https://www.echa.europa.eu/web/guest/registration-dossier/-/registered-dossier/16012
ECHA (2017): HFO-1234ze substance information. Available at: https://www.echa.europa.eu/web/guest/substance-information/-/substanceinfo/100.104.972?_disssubsinfo_WAR_disssubsinfoportlet_backURL=https%3A%2F%2Fwww.echa.europa.eu%2Fweb%2Fguest%2Fhome%3Fp_p_id%3Ddisssimplesearchhomepage_WAR_disssearchportlet%26p_p_lifecycle%3D0%26p_p_state%3Dnormal%26p_p_mode%3Dview%26p_p_col_id%3Dcolumn-2%26p_p_col_pos%3D1%26p_p_col_count%3D7%26_disssimplesearchhomepage_WAR_disssearchportlet_sessionCriteriaId%3D
ECHA (2017): HCFO-1234zd substance information. Available at: https://echa.europa.eu/substance-information/-/substanceinfo/100.149.148

HFO-1234yf health hazards

It is important to note, that ECHA have performed checks on the REACH dossier for HFO-1234yf and made evaluation decisions. The decision to ask the applications to conduct a 90-day repeated acute toxicity study in the rabbit by inhalation was annulled by the Board of Appeal (ECHA, 2013). ECHA in 2015 requested an updated Chemical Safety Report (CSR) with revised DNELs for workers and also a revised exposure assessment for inhalation and risk characterisation for workers or to justify why recommended assessment factors in DNEL derivation were not used (ECHA, 2015). Based on the substance evaluation on HFO-1234yf by Baua (Germany), more information on the mutagenicity of the substance has been requested (European Commission, 2015).

HFO-1234yf is presently not classified as acutely toxic and no acute Derived No Effect Level (DNEL) is therefore appropriate. HFO-1234yf by inhalation exposure is poorly adsorbed, undergoes minimal metabolism, and is rapidly cleared from the body; it will not bioaccumulate. In addition, no systemic toxicity was observed in following repeated exposure and no genotoxicity was observed following *in vivo* exposure. It is not considered an acute inhalation hazard based on an inhalation 4 hr LC_{50} (lethal concentration that causes death in 50% of the subjects) of 400,000 ppm and the absence of cardiac sensitisation at the highest concentration tested (120,000 ppm). For the worker DNEL systemic exposure, the German MAK (Maximum Concentration at the Workplace) value of 950 mg/m^3 (200 ppm) is used (MAK Collection, 2015). For the MAK value, data was used from animal studies due to the lack of human health data (ECHA, 2017a). Under the SNAP (Significant New Alternatives Policy) program, HFO-1234yf for its approved uses does not have a significantly greater impact on human health than the use of other available substitutes (US Environmental Protection Agency, 2015).

HFO-1234ze health hazards

As for HFO-1234yf, information on the health hazards from exposure to HFO-1234ze is limited. The REACH dossier states that HFO-1234ze is poorly absorbed, will undergo minimal metabolism and will be cleared rapidly from the body (ECHA, 2017b). HFO-1234ze has also been considered to pose no greater overall risk to human health than other alternatives (US Environmental Protection Agency, 2010).

HFO-1233zd health hazards

In the REACH dossier, no health hazards were identified (ECHA, 2017c) with the basis of the hazards from a study on rats. US EPA lists the following possible side effects for this substance (US Environmental Protection Agency, 2014):

- Serious eye irritation;
- Skin irritation;
- Frostbite;
- Potential for central nervous system effects for example drowsiness and dizziness; and
- Asphyxiation in confined spaces

HFO blends health hazards

HFO blends have similar health hazards to that of the pure HFO substance. For example, HFO blend R-452A (Opteon™ XP44) is listed in its safety data sheet as being an asphyxiant in high concentrations and contact with the evaporating liquid can cause frostbite or freezing of the skin (BOC, 2014). HFO blend R-448A (Solstice® N40) is also listed as a possible skin or eyes irritant, can cause frostbite, at high concentrations can cause an irregular heartbeat and cause as asphyxiation in confined spaces.

These effects are listed as being common for many refrigerants (US Environmental Protection Agency, 2014).

7.2 Workers health and safety

7.2.1 Overview

Literature review and consultation have identified that manufacturing workers, refrigerant workers (such as technicians and repair workers) and recyclers may be potentially exposed to HFOs. This section describes the processes involved, risk management measures in place and elevated levels and/or leaks of HFOs for workers' health and safety. Information about ECHA's comments on workers' health for the REACH registration dossier is discussed in Section 7.1.

7.2.2 Manufacturing workers

Exposure

From consultation with a major HFO manufacturer, the production of HFOs is a closed process with a limited number of workers potentially exposed (process is illustrated in the below figure).

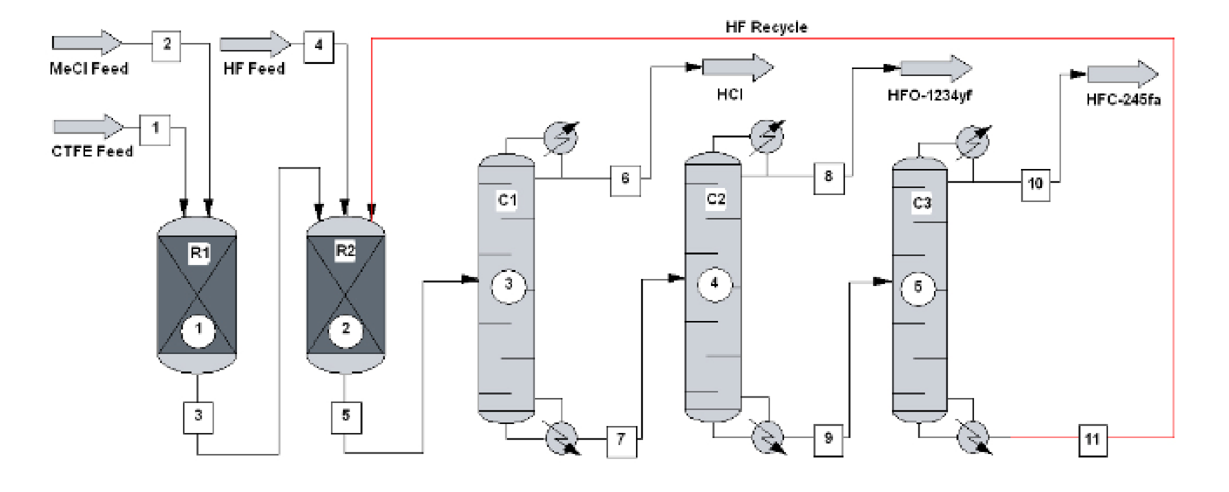


Figure 7-1: Production process for HFO-1234yf
Source: ICTT (2013): Upstream climate impacts from production of R-134A and R-1234yf refrigerants used in mobile air conditioning systems. Available at: http://www.theicct.org/publications/upstream-climate-impacts-r-134a-and-r-1234yf

Workplace exposure is also monitored by independent hygiene specialists and also by use of sensors. Workplace concentrations from air sampling performed by the manufacturer have resulted in concentrations between 0 and 1 ppm (this is also required for registration with the US EPA). The REACH dossiers also include information on the uses at industrial sites and by professional workers which is summarised in the table overleaf.

Table 7-2: Uses of HFOs at industrial sites (such as manufacturing workers)

HFO	Processes by professional workers and at industrial sites
HFO-1234yf	PROC 8a: Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at non-dedicated facilities; PROC 8b: Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at dedicated facilities; and PROC 9: Transfer of substance or preparation into small containers (dedicated filling line, including weighing)
HFO-1234ze	PROC 8a: Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at non-dedicated facilities for the servicing of air conditioning and refrigeration systems; PROC 9: Transfer of substance or preparation into small containers (dedicated filling line, including weighing) for the manufacture of air conditioning and refrigeration systems
HFO-1233zd	PROC 8a: Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at non-dedicated facilities for the servicing of air conditioning and refrigeration systems; PROC 9: Transfer of substance or preparation into small containers (dedicated filling line, including weighing) for the manufacture of air conditioning and refrigeration systems

Sources: ECHA (2017): Polyhaloalkene registration dossier. Available at: https://www.echa.europa.eu/web/guest/registration-dossier/-/registered-dossier/16012
ECHA (2017): HFO-1234ze Substance Information. Available at: https://www.echa.europa.eu/web/guest/substance-information/-/substanceinfo/100.104.972?_disssubsinfo_WAR_disssubsinfoportlet_backURL=https%3A%2F%2Fwww.echa.europa.eu%2Fweb%2Fguest%2Fhome%3Fp_p_id%3Ddisssimplesearchhomepage_WAR_disssearchportlet%26p_p_lifecycle%3D0%26p_p_state%3Dnormal%26p_p_mode%3Dview%26p_p_col_id%3Dcolumn-2%26p_p_col_pos%3D1%26p_p_col_count%3D7%26_disssimplesearchhomepage_WAR_disssearchportlet_sessionCriteriaId%3D
ECHA (2017): HCFO-1234zd Substance Information. Available at: https://echa.europa.eu/substance-information/-/substanceinfo/100.149.148

Occupational exposure levels (OELs) have been set by the Workplace Environment Exposure Level (WEEL) committee with an OEL of 800 ppm (400 ppm for an 8 hour time weighted average) for HFOs generally and for HFO-1234ze, the OEL is 1000 ppm.

7.2.3 Refrigerant workers

An association confirmed that HFOs and HFO/HFC blends have been evaluated as alternative refrigerants with GWP in accordance with F-gas requirements and are subject to F-gas Regulations. Refrigerant workers (such as refrigerant manufacturers and repair technicians) also need to be considered for workers' health and safety for HFO refrigerants.

Under both the ODS and F-gas regulation in the EU, technicians need to undergo training and certification. For handling HFOs, under the F-gas regulation:

- In Annex II of the 2014 F-Gas Regulation Lists the familiar HFOs and notes that they are subject to reporting under Article 19;
- The text on Containment (Article 3), Leak Checks (Article 4) and Leak Detection Systems (Article 5) all refer to 'fluorinated greenhouse gases'; and
- In Article 10 on Training and Certification relates to Equipment types (as listed in Article 4(2)) not refrigerant types. Hence, engineers need to be certified irrespective of the refrigerant type.

For stationary refrigeration and air conditioning, this is required for installation, leakage checking, maintenance or servicing, refrigerant recovery and decommissioning (Gluckman Consulting, 2016a). For mobile air conditioning (MAC), all technicians that are involved in F-gas recovery which is defined under the scope of the MAC directive are required to undergo training (Gluckman Consulting, 2016b). In the United States, refrigerant technicians are also required to undergo certification for mobile air conditioning applications (US Environmental Protection Agency, 2017).

The Federation of Environmental Trade Associations (FETA) also supplies general guidelines for refrigerant technicians (FETA, 2015). Technicians who perform work for stationary RACHP (Refrigeration, Air-Conditioning and Heat Pumps) systems must possess an F-gas handling certificate. The work area should also be well ventilated with fans or blowers used in confined areas for the dispersion of vapours, the available oxygen in the area should be tested (not using a leak monitor), and an A2L (mildly flammable refrigerants) flammable rated refrigerant leakage detector and equipment for monitoring oxygen should be installed in the work areas.

For maintenance and end-of-life recovery, consultation indicated that for recovery of refrigerants (used in closed high pressure systems), minimising the workers exposure to below the OEL, the process is as follows:

- Special equipment is connected to the recovery cylinder;
- The valve is opened;
- The material is recovered;
- The valve is closed; and
- The recovered material is taken away

In the case of HFO-1234yf, in the REACH registration dossier (ECHA, 2017a) worker activity related to installation, servicing and maintenance is covered by the exposure scenarios which are used for industrial workers (for example, see Table 7-2).

Recycling and reclamation workers

Recycling and reclamation workers also need to undergo relevant F-gas training. From consultation with a reclaimer, if the recovered refrigerant material is not suitable for re-processing, the material must be treated at an approved waste treatment facility. This would typically involve high temperature incineration with scrubbing and neutralisation controls to reduce exposure for workers and the environment (the use of a wet scrubber typically has a 50-70% efficiency for reducing exposure to the environment from the European Chemical Industry Council (Cefic) RMM library) (Cefic, undated).

7.2.4 Risk management measures

Risk Management Measures (RMM) have been discussed in Section 7.1 for manufacturing and refrigeration workers in terms of the process involved, for example the use of closed systems and training.

As well as the use of closed processes, other engineering measures and the use of Personal Protection Equipment (PPE) is recommended for workers handling HFOs. These are discussed in following tables and where appropriate the efficiency of the measures to reduce workplace exposure has been analysed using the Cefic RMM library (Cefic, undated).

Table 7-3: HFO-1234yf risk reduction measures		
Measure	**Details**	**Efficiency**
Engineering measure	Use highly effective exhaust ventilation	Local exhaust ventilation (LEV) has an 80% inhalation efficiency
Respiratory protection	Wear suitable respiratory equipment (meets EN 136, 140, 149 standards) if ventilation is insufficient	Full face masks (EN 136) can have an inhalation efficiency of 75-97.5% depending on mask chosen; Half face masks (EN 140): 75-95% can have an inhalation efficiency of 75-95% depending on mask chosen
Hand protection	Wear suitable gloves (EN 374 standard) and use heat insulating gloves	N/A (The efficiency for chemical resistant gloves is expressed in duration of protection before permeation occurs; no data is available for HFOs)
Eye protection	Wear googles (EN 166 standard)	N/A
Skin and body protection	Wear suitable personal protection equipment	N/A (The efficiency for chemical resistant clothing, boots is expressed in duration of protection before permeation occurs)
Protective measures	PPE to be used. Protective suit must meet standards EN 340, 463, 468, 943-1, 943-2. Safety shoes must meet EN-ISO 20345 standard	N/A
Sources: Cefic (undated): RMM Library. Available at: www.cefic.org/Documents/...and.../Risk%20Management%20Measures%20(RMM).xls ECHA (2017a): Polyhaloalkene registration dossier. Available at: https://www.echa.europa.eu/web/guest/registration-dossier/-/registered-dossier/16012 Honeywell (2017): Solstice® yf Refrigerant (R-1234y). Available at: http://msds-resource.honeywell.com/ehswww/hon/result/result_single_main.jsp?C001=MSDS&C102=GB&C101=SDS_GB&C100=E&P_LANGU=E&C013=&C997=C100;E%2BC101;SDS_GB%2BC102;GB%2B1000&P_SYS=1&C008=&C006=HON&C005=000000011078&		

Table 7-4: HFO-1234ze risk reduction measures		
Measure	**Details**	**Efficiency**
Engineering measure	Use local exhaust ventilation	Local exhaust ventilation (LEV) has an 80% inhalation efficiency
Respiratory protection	Wear suitable respiratory equipment (positive-pressure supplied air respirator) if ventilation is insufficient	Inhalation efficiency of 90-95% depending on mask chosen
Hand protection	Use heat insulating gloves (Viton)	N/A (The efficiency for chemical resistant gloves is expressed in duration of protection before permeation occurs; no data is available for HFOs)
Eye protection	Wear googles	N/A
Skin and body protection	Wear impervious clothing (cold insulating gloves/face shield/eye protection)	N/A (The efficiency for chemical resistant clothing, boots is expressed in duration of protection before permeation occurs)
Sources: Cefic (undated): RMM Library. Available at: www.cefic.org/Documents/...and.../Risk%20Management%20Measures%20(RMM).xls ECHA (2017): HFO-1234ze registration dossier. Available at: https://echa.europa.eu/registration-dossier/registered-dossier/15736/		

Table 7-5: HFO-1233zd risk reduction measures		
Measure	**Details**	**Efficiency**
Engineering measure	Use local exhaust ventilation; perform filling operations only at stations with exhaust ventilation facilities	Local exhaust ventilation (LEV) has an 80% inhalation efficiency in reducing exposure
Respiratory protection	Wear suitable respiratory equipment if ventilation is insufficient	Respiratory equipment can have an inhalation efficiency of 75%-97.5% depending on equipment chosen
Hand protection	Use gloves (Viton (R) Vitoject 890)	N/A (The efficiency for chemical resistant gloves is expressed in duration of protection before permeation occurs; no data is available for HFOs)
Eye protection	Wear googles	N/A
Skin and body protection	Use protective footwear	N/A
Sources: Cefic (undated): RMM Library. Available at: www.cefic.org/Documents/...and.../Risk%20Management%20Measures%20(RMM).xls ECHA (2017): HFO-1233zd registration dossier. Available at: https://echa.europa.eu/registration-dossier/-/registered-dossier/10762/1 Honeywell Refrigerants (2017): Solstice® zd. Available at https://www.honeywell-refrigerants.com/americas/product/solstice-zd/		

Table 7-6: HFO blends risk reducing measures (HFO blend 452A)		
Measure	**Details**	**Efficiency**
Engineering measure	Consider the use of a work permit system; ensure adequate ventilation; check pressurised systems for leaks; use permanent leak tight connections; use oxygen detectors	N/A
Respiratory protection	Not required	N/A
Hand protection	Use gloves (EN 388 standard)	N/A (The efficiency for chemical resistant gloves is expressed in duration of protection before permeation occurs; no data is available for HFOs)
Eye protection	Use Safety eyewear, goggles or face shield (EN166 standard)	N/A
Skin and body protection	Use protective footwear	N/A
Sources: BOC (2014): Safety Data Sheet Opteon XP 44. Available at: https://www.boconline.co.uk/internet.lg.lg.gbr/en/images/Refrigerant-R-452A-XP44-10022546410_139210.pdf?v=3.0		

7.2.5 Accidental release and elevated levels and/or leaks of HFOs

The literature review has identified a lack of available studies on workers' health to elevated levels of HFOs. The main source of information has been REACH registration dossiers and material safety data sheets which discuss accidental release measures for accident release and/or leaks of HFOs. No studies have been identified from literature review and consultation for the effect to human health from elevated HFO levels and/or HFO exposure. For leakages, levels of a maximum of 1 ppm have been measured at pipes (source of leakage) by an HFO manufacturer.

Accidental release measures recommendations are as follows for HFO-1234yf (ECHA, 2017a, Honeywell 2017):

- Full protective clothing and self-contained breathing apparatus are to be used;
- People are to be kept away from the leak/spill and also upwind of the leak/spill;
- The area of the leak/spill is to be ventilated;
- For cleaning the leak/spill explosion-proof electrical equipment and/or low sparking hand tools should be used and the leak/spill allowed to evaporate;
- Prevent the substance from entering drains;
- Pay attention to the spreading of the gas particularly at ground level and also pay attention to the wind direction; and
- Inform the responsible authorities if there is a gas leakage, entry into soil or drains or entry into waterways.

DuPont (DuPont, 2012) also recommend that for leaks, nearby electricity sources may produce an undesirable spark and that power should be interrupted at a remote location from the leak. For areas where leaks occur, mechanical ventilation should be provided.

From information gathered during consultation with a manufacturer, established guidelines based on industrial hygiene regulations, for example, the guidelines of the European Agency for Safety and Health at work, are followed for accidental release or leaks. Furthermore, the consultation revealed that workers are exposed to HFO levels far below the OELs and if a worker was exposed to levels above the OEL they would be taken out of the process and given sufficient ventilation and aspiration.

HFO-1234yf and HFO-1234ze also have available refrigeration concentration levels of 0.058 kg/m^3 and 0.061 kg/m^3 respectively; a Quantity Limit with Minimal Ventilation (QLMV) of 0.060 kg/m^3 and 0.063 kg/m^3 respectively; and a Quantity Limit with Adequate Ventilation (QLAV) of 0.14 kg/m^3 and kg/m^3 respectively (FETA, 2015).

7.2.6 Fire/explosion products and impact on workers' health and safety

The fire/explosion products for HFOs and HFO/HFC blends that have been identified as being used as refrigerants are summarised in the table overleaf. Generally, the decomposition products are as follows (note these equations are not balanced and are shown for clarity):

$C_3H_2F_4$ (HFO-1234yf and HFO-1234ze) → $COF_2 + CO_x$ + HF + others (1)

$C_3H_2F_3Cl$ (HFO-1233zd) → CO + CO_2 + -C(=O) X (X=halide) +HCl +HF (2)

HFO blends ($C_3H_2F_4$ based) → CO_x + HF + COF_2 + C_xF_y (3)

where COF_2 is carbonyl fluoride; COx is carbon oxides; CO is carbon monoxide; HF is hydrogen fluoride; C(=O) X are carbonyl halides; HCl is hydrochloric acid; and C_xF_y are fluorocarbons.

Table 7-7: Thermal (fire/explosion) decomposition products of HFOs	
HFO	**Decomposition products**
HFO-1234yf	Carbonyl fluoride (COF_2), carbon oxides (CO_x), hydrogen fluoride (HF), fluoride pyrolysis products
HFO-1234ze	Carbon monoxide (CO), carbon dioxide (CO_2), carbonyl halides, hydrogen halides and pyrolysis products that contain fluorine
HFO-1233zd	Carbon monoxide, carbon dioxide, carbonyl halides, gaseous hydrogen chloride (HCl) and gaseous hydrogen fluoride
Blends (HFO-1234yf based blends)	Carbon oxides, fluorocarbons, hydrogen fluoride and carbonyl difluoride
Sources: BOC (2014): Safety Data Sheet Opteon XP 44. Available at: https://www.boconline.co.uk/internet.lg.lg.gbr/en/images/Refrigerant-R-452A-XP44-10022546410_139210.pdf?v=3.0 BOC (2015): Safety Data Sheet Opteon XP 40. Available at: https://www.boconline.co.uk/internet.lg.lg.gbr/en/images/Refrigerant-R449A-10022608410_168682.pdf?v=4.0 ECHA (2017): HCFO-1234zd registration dossier. Available at: https://echa.europa.eu/registration-dossier/-/registered-dossier/10762 ECHA (2017): Polyhaloalkene registration dossier. Available at https://www.echa.europa.eu/web/guest/registration-dossier/-/registered-dossier/16012 Honeywell (2017): Solstice® yf Refrigerant (R-1234y). Available at: http://msds-resource.honeywell.com/ehswww/hon/result/result_single_main.jsp?C001=MSDS&C102=GB&C101=SDS_GB&C100=E&P_LANGU=E&C013=&C997=C100;E%2BC101;SDS_GB%2BC102;GB%2B1000&P_SYS=1&C008=&C006=HON&C005=000000011078& Honeywell (2017): Solstice® ze Refrigerant Safety Data Sheet. Available at https://msds-resource.honeywell.com/ehswww/hon/result/result_single.jsp?P_LANGU=E&P_SYS=1&C001=MSDS&C997=C100%3BE%2BC101%3BSDS_GB%2BC102%3BGB%2B1000&C100=*&C101=*&C102=*&C005=000000016095&C008=&C006=HON&C013=+	

Carbonyl fluoride (COF_2) is a toxic gas that can be very toxic through inhalation, can cause severe burns and eye damage, and causes damage to organs (PubChem, undated). Carbonyl fluoride is also hydrolysed to hydrogen fluoride (HF) which can be toxic by inhalation (Tsai, 2005). Carbonyl fluoride is short lived; however, exposure could still occur.

Hydrogen fluoride (HF) is an extremely toxic gas and exposure can occur via the inhalation or dermal route. Dermal contact occurs mainly in an occupational setting) and can cause severe skin burns, whilst exposure to high levels can cause lung and heart damage and in extreme cases, death (SEPA, undated). Tests performed by JRC (Joint Research Centre, 2014) found no HF above concentrations of 1 ppm at high ignition temperatures in refrigerant release tests. Greenpeace in their HFO position paper (Greenpeace, 2016) have also expressed concern over the potential formation of HF from the combustion of HFOs. Further information on HF and its environmental effects are discussed in section 6.3.

DuPont (DuPont, 2012) state that for HFO-1234yf, fire or explosion may occur if the concentration of vapour in the air are within the flammable range of the substance and an adequate energy level ignition source is available (potential ignition sources should be kept away from equipment with HFO-1234yf) and also HFO-1234yf should not mixed with air, oxygen or other oxidisers above atmospheric pressure. HFO-1234yf also has an auto ignition temperature of 405 °C (DuPont, 2012).

The JRC of the European Commission has studied the ignition of HFO-1234yf refrigerants in vehicles (Joint Research Centre, 2014). No refrigerant ignitions occurred at high engine compartment temperatures and refrigerant ignition only occurred at extreme conditions and involved combining elements that were unlikely to occur. JRC also discuss results from a report by KBA (Kraftfahrt Bundesamt) and other studies where refrigerant ignition only occurred above 700 °C. From consultation, in the case of combustion there is also convection which would result in combustion going up into the air whilst HFO emissions in fires have not been measured.

Following on from this, the combustion of HFO-1234yf has recently been studied (Magnusson et al, 2016) in small scale laboratory combustion experiments. From the combustion experiments, almost a quarter to half of the HFO-1234yf remained unreacted, with carbonyl fluoride, carbon dioxide, hydrogen fluoride and water the major combustion products. Saturated and unsaturated fluorocarbons were also emission products at lower concentrations. The full list of products formed and their concentrations are listed in the below table.

Table 7-8: Combustion products of HFO-1234yf

Chemical Compound	Chemical formula	Emission factor [mg/g fuel]
HFO-1234yf		220-480
Carbonyl fluoride	COF_2	170-360
Carbon dioxide	CO_2	120-320
Hydrogen fluoride	HF	70-240
Water	H_2O	60-170
Carbon monoxide	CO	5-80
Hexafluoroethane	C_2F_6	15-33
Tetrafluoromethane	CF_4	6-24
1,1-Difluoroethene	C_2F_2H	2.4-6.6
Trifluoromethyl acetylene	C_2F_3H	0.2-2
Pentafluoroethane	C_2F_5H	0.6-1.6
Trifluoromethane	CF_3H	0.6-1.4
Fluoroethene	C_2FH_3	0.5-1.2
1,1,1,2-Tetrafluoroethane	$C_2F_4H_2$	0.7-1.1
1,1,2,2,2-Pentafluro-1-propene	C_3F_5H	0.2-1
Octafluoropropane	C_3F_8	0.3-0.9
Tetrafluoroethene	C_2F_4	0.2-0.8
Trifluoroethene	C_2F_3H	0.2-0.5
1,1,1,3,3,3-Hexafluoropropane	C_3F_6	0.2-0.4
3,3,3-Trifluropropene	$C_3F_3H_3$	0.1-0.4
Hexafluoropropene	C_3F_6	0.04-0.3
Acetylene	C_2H_2	0.08-0.27
Bis(trifluoromethyl)acetylene	C_4F_6	0.03-0.2
1,1,1-Trifluoroethane	$C_2F_3H_3$	0.04-0.08
1,2-Difluoroethene	$C_2F_2H_2$	<0.06
Non identified compounds (six non identified compounds)	-	2.5-3.9

Source: Magnusson, R. et al (2016): Identification and brief toxicological assessment of combustion products of the refrigerant HFO-1234yf. Available at: https://www.t-olycka.se/index.php/files/17/Bilbraender/401/foir4285.pdf

8 Risk assessment

8.1 Overview

This section describes the results of the risk assessment performed for HFO refrigerant use up to the year 2100, using the projected emissions from the MIT-5 approach (Section 4). As part of this section, the inputs/outputs for the EUSES model are described and the assumptions that have been made for the model are discussed. TFA has been modelled as the decomposition product of HFO-1234yf. The results and conclusions are also discussed.

It should be noted that TFA is a REACH registered substance with a harmonised CLP classification as indicated below:

Table 8-1: CLP classification of TFA

Hazard Class and Category Code	Hazard Statement Code	Hazard Statement language
Skin Corrosive 1A	H314	Causes severe skin burns and eye damage
Acute Toxic 4	H332	Harmful if inhaled
Aquatic Chronic 3	H412	Harmful to aquatic life with long lasting effects

However, ECHA (2017e) have requested that the lead registrant for TFA to submit requested information, which is summarised below, in an updated registration dossier by 7 January 2021, except for the information requested under point 1 for a sub-chronic toxicity study (90-day) which shall be submitted in an updated registration dossier by 9 July 2018.

1. *'Sub-chronic toxicity study (90-day), oral route (Annex IX, Section 8.6.2.; test method: EU B.26./OECD TG 408) in rats with the registered substance adjusted to physiological pH;'*

The study records, provided by the registrant does not provide the information required by Annex IX,Section 8.6.2., because exposure duration is less than 90 days and not all tissues/organs are histopathologically investigated and would not necessarily have the same statistical power as a study according to OECD TG 408 would require. Therefore, ECHA states that the information provided on this endpoint for the registered substance in the technical dossier does not meet the information requirement. Consequently, there is an information gap and it is necessary to provide information for this endpoint.

2. *'Pre-natal developmental toxicity study (Annex IX, Section 8.7.2.; test method: EU 8.3I./OECD TG 414) in a first species (rat or rabbit), oral route with the registered substance adjusted to physiological pH.'*

ECHA highlight that the registrant provided study records for three non-guideline studies, that there are methodological deficiencies in the studies and more specifically and these studies do not cover key parameters of pre-natal developmental toxicity effects *in vivo*. Therefore, ECHA states that the individual sources of information in the dossier do not provide the information required for this endpoint.

3. *Pre-natal developmental toxicity study (Annex X, Section 8.7.2.; test method: EU 8.3I./OECD TG 414) in a second species (rabbit or rat), oral route with the registered substance adjusted to physiological pH;'*

ECHA highlights that there is no information provided for a pre-natal developmental toxicity study in a second species. Therefore, the information provided on this endpoint for the registered substance in the technical dossier does not meet the information requirement. Consequently, there is an information gap and it is necessary to provide information for this endpoint.

4. *'Extended one-generation reproductive toxicity study (Annex X, Section 8.7.3.; test method: EU 8.56./OECD TG 443) in rats, oral route with the registered substance adjusted to physiological pH, specified as follows:*

   - Ten weeks premating exposure duration for the parental (PO) generation;
   - Dose level setting shall aim to induce some toxicity at the highest dose level;
   - Cohort 1A (Reproductive toxicity);
   - Cohort 1B (Reproductive toxicity) without extension to mate the Cohort 18 animals to produce the F2 generation.'

ECHA considers that there is not sufficient weight of evidence from several independent sources of information which would allow it to assume/conclude that the substance does not have a particular dangerous property, i.e. reproductive toxicity. Therefore, ECHA concludes that the information provided on this endpoint for the registered substance in the technical dossier does not meet the information requirement. Consequently, there is an information gap and it is necessary to provide information for this endpoint.

5. *'Identification of PNEC and risk characterisation (Annex I, Section 3.3.1. and 6.): revise PNECs for freshwater, marine water, freshwater sediment and marine sediment using the study giving rise to the highest concern according to Annex I, Section 3.1.5 and revise the risk characterisation accordingly or provide a detailed justification for not using the recommendations of ECHA guidance in PNEC derivation.'*

ECHA highlights issues with the way the PNEC values have been calculated and the lead registrant has been requested to revise PNECs for freshwater, marine water, freshwater sediment, marine sediment using the result giving rise to the highest concern, i.e. the NOEC of O.2 mg/L for *Raphidocelis subcapitata* (formerly known as *Selenastrum capricornutum and Pseudokirchneriella subcapitata*).

6. *'Exposure assessment and risk characterisation (Annex I, Sections 5. and 6.) for environment.*
   - Revise the exposure assessment to provide a detailed justification' including related risk management measures, for using non-default release factor in the exposure estimation for exposure scenarios ESl and ES2 or to apply default release factors according to ECHA Guidance R.16.
   - Revise the exposure assessment to apply a "fraction of the main source" of 100% for exposure scenarios ES3, ES4 and ES6 in accordance with the recommendations of ECHA Guidance R.16 or to provide adequate justification for any deviation from these recommendations.
   - The risk characterisation shall be revised accordingly.'

ECHA indicates that there is missing information on the risk management measures for the manufacture of TFA on the plant (next words blocked out) and there are deviations on the assumed fraction used at main source (i.e. annual use amount at a site).

7. *'Exposure assessment (Annex I, Section 5.1.1.) for human health: provide documentation for the recommended personal protective equipment, i.e. hand and skin protection, respiratory protection and eye/face protection;*
   - specify the type of glove material, thickness and breakthrough times;

- specify the filter type/class for the respiratory protective
- specify the type and quality of protective clothing.'

ECHA highlights that the specific detailed information on the recommended personal protective equipment (PPE) is missing from both from the CSR and from the information on safe use within the IUCLID dossier. ECHA have requested the registrant provide more detailed information on the PPE above.

It is suggested that these developments for the TFA REACH registration dossier are followed.

8.2 VEGA results

Selected results of the prediction of the properties TFA from its structure using VEGA are discussed in the following table. The full VEGA output is included in Annex 3. It should be noted, that these results are only indicative and would require further investigation.

Table 8-2: VEGA results for TFA

Test	Prediction	Comment
Mutagenicity	Non-Mutagen	Low-moderate-high reliability, models all suggest non-mutagenicity
Carcinogenicity	Possible non-carcinogen	Uncertain, low-moderate reliability carcinogenicity and non-carcinogenicity is indicated
Developmental toxicity and estrogen receptor binding	non-toxicity and non-active	Low reliability
Skin sensitizer	Non-sensitizer	Moderate reliability
Eco-toxicity: fish and crustacean	Non-toxicant (both)	Moderate reliability
BCF	Non-bioaccumulative	Low-moderate reliability
Log P_{ow}	Non-bioaccumulative	High-moderate reliability
Biodegradable	Non readily biodegradable	Low-moderate-high reliability

8.2.1 VEGA prediction and applicability domain comments

For all models the predictions were based on six similar compounds; however the compounds were identified as being moderately similar and not necessarily optimal for the models. Some of the experimental results also disagreed with some of the predicted values. Also, some of the compounds used in a model were also used in a model which predicted the same and different endpoints. High reliability is expected to be within the applicability domain of the model, moderate reliability could be could be out of the applicability domain of the model and low reliability is expected to be outside the applicability domain of the model.

Attempts to generate additional QSAR information (and read across) for the physical chemical properties, environmental fate and transport, ecotoxicological information and human health hazard potential of TFA could be investigated using the OECD QSAR Toolbox, EPI Suite and other QSAR software.

Mutagenicity

A total of five mutagenicity models were run in VEGA (with some crossover):

- CONSENSUS 1.0.1 produced a consensus score of 0.47 (non-mutagenic);
- CAESAR 2.1.13 predicted non mutagenicity (high reliability);
- SarPy/IRFMN 1.0.7 predicted non mutagenicity (moderate reliability);
- ISS 1.0.2 predicted non mutagenicity (low reliability); and
- KNN/Read-Across 1.0.0 predicted non mutagenicity (low reliability).

Carcinogenicity

A total of four carcinogenicity models were run in VEGA:

- CAESAR 2.1.9 predicted carcinogenicity (low reliability);
- ISS 1.0.2 predicted non-carcinogenicity (low reliability);
- IRFMN/Antares 1.0.0 predicted carcinogenicity (moderate reliability); and
- IRFMN/ISSCAN-CGX 1.0.0 predicted possible non-carcinogenicity (low reliability).

Developmental toxicity and estrogen receptor binding

A total of two developmental/reproductive toxicity models and two estrogen receptor binding models were run in VEGA:

- CAESAR 2.1.7 predicted non-toxicity (low reliability);
- Toxicity library (PG) 1.0.0 predicted non-toxicity (low reliability);
- Estrogen Receptor Relative Binding Affinity model (IRFMN) predicted inactive (low reliability); and
- Estrogen Receptor-mediated effect (IRFMN/CERAPP) 1.0.0 predicted possible non-active (high reliability).

Skin sensitizer

One skin sensitizer model was run in VEGA:

- CAESAR 2.1.6 predicted non-sensitizer (moderate reliability)

Toxicity

Fish Acute toxicity

A total of four models were run in VEGA:

- SarPy/IRFMN 1.0.2 predicted non-toxic (moderate reliability);
- KNN/Read-Across 1.0.0 predicted toxicity of 177.19 mg/L (moderate reliability);
- NIC 1.0.0 predicted toxicity of 244.67 mg/L (moderate reliability); and
- EPA 1.0.7 predicted toxicity of 290.52 mg/L (moderate reliability).

Daphnia Magna toxicity

A total of 2 models were run in VEGA:

- EPA 1.0.7 predicted toxicity of 56.96 mg/L (moderate reliability); and
- DEMETRA 1.0.4 predicted toxicity of 180.87 mg/L (moderate reliability).

Bee

No predictions for bees were possible in VEGA.

BCF model

A total of three models were run in VEGA:

- CAESAR 2.1.14 predicted low bioaccumulation (0.2 log(L/kg)) (moderate reliability);
- Meylan 1.0.3 predicted low bioaccumulation (0.5 log(L/kg)) (low reliability); and
- KNN/Read-Across 1.1.0 predicted low bioaccumulation (0.27 log(L/kg)) (low reliability).

Log P_{ow}

A total of three models were run in VEGA:

- Meylan/Kowwin 1.1.4 is predicted to be non-bioaccumulative (Log P: 0.5) (high reliability);
- MLogP 1.0.0 is predicted to be non-bioaccumulative (Log P: 0.37) (high reliability); and
- ALogP 1.0.0 is predicted to be non-bioaccumulative (Log P: 0.86) (moderate reliability).

Biodegradable

A total of four models were run in VEGA:

- Ready Biodegradability model IRFMN 1.0.9 predicted non-readily biodegradable (moderate reliability);
- Persistence (sediment) model IRFMN 1.0.0 predicted non-persistence (low reliability);
- Persistence (soil) model IRFMN 1.0.0 predicted non-persistence (high reliability); and
- Persistence (water) model IRFMN 1.0.0 predicted non-persistence (moderate reliability).

8.3 EUSES model inputs

The EUSES model is primarily used for non-polar organic compounds; however EUSES has been used to perform risk assessments for inorganic compounds and other substances. Suggestions for how to deal with difficult substances in EUSES have been recommended (RIVM, 2000), while the contributors to the development of the EUSES model have recognised that improvements could be made to the model and have suggested updates that should be made to EUSES (RIVM, 2014). For example, this includes suggestions for acid dissociation constants (pK_a).

TFA posed a challenge principally as if more additional data was available this would have allowed for a more complete prediction of the environmental and human health risks of TFA. Also, HFO-1234yf is the parent compound that is being produced and the one that will be emitted, whereas TFA is the breakdown substance. The breakdown of HFO-1234yf to TFA will usually occur in the atmosphere, away from the other sources of distribution which is the case for other substances (e.g. emission directly to wastewater and surface water). Assuming that a higher fraction of release and emission to air of TFA may lead to inaccurate RCR values for soil. The outputs of this model should therefore be used with caution.

For the EUSES model inputs (for the EU), information has been provided from the REACH registration dossier (ECHA, 2017d) for TFA, the Sigma Aldrich Safety Data Sheet (SDS) for TFA (Sigma Aldrich, 2017) and other information sources which are indicated where relevant. An example of the inputs for the risk assessment is provided in Annex 1. Assumptions are also stated where these have been made for the input information. Default values available in EUSES have also been utilised and these are stated where used. The inputs used in the risk assessment model are discussed in the following sections.

8.3.1 Assumptions and potential issues

A number of assumptions have had to be made during the EUSES process; a precautionary approach has been used which represents a worst case scenario. This includes the following:

- The toxicity value for microorganisms is lower (i.e. more toxic) than that of (some) aquatic species, 832 mg/L in OECD 209 test compared to 1,200 mg/L in most aquatic toxicity tests; and
- Also, the LC_{50} test result for plants of 250 mg/kg dwt is lower than both of these toxicity values.

This could be leading to the Risk Characterisation Ratio (RCR) values for sediment and the sewage treatment plants to be higher than expected. It would anticipate that these have been overestimated, perhaps by an order of magnitude. The reason for this is that from information obtained for Parts 1 and 2 of the study, HFO's are gases and when emissions occur they will be transported. HFOs are more likely to be used and manufactured in urban or close to urban environments, however when emissions occur they will be transported away from these environments where they will breakdown in TFA and therefore TFA will be deposited in a different environment, an environment that may not be connected to STPs.

8.3.2 Physico-chemical properties

The physio-chemical properties that have been used for TFA for the model are described in the below table.

Table 8-3: Physico-chemical properties	
Molecular Weight	114.02
Melting point	-15.2 °C
Boiling point	71.78 °C
Vapour Pressure	15800 Pa (25°C)
Water solubility	1E+05 (set to maximum)
Octanol-water partition coefficient	-0.2
Sources: ECHA (2017): Trifluoroacetic acid registration dossier. Available at: https://echa.europa.eu/registration-dossier/-/registered-dossier/5203/6/1and Sigma Aldrich (2017): Trifluoroacetic acid SDS. Available at: https://www.sigmaaldrich.com/MSDS/MSDS/DisplayMSDSPage.do?country=GB&language=en&productNumber=T62200&brand=SIAL&PageToGoToURL=https%3A%2F%2Fwww.sigmaaldrich.com%2Fcatalog%2Fproduct%2Fsial%2Ft62200%3Flang%3Den	

Partition coefficients and bioconcentration factors

The partition coefficients and bioconcentration factors that have been used for TFA are discussed in the overleaf table.

Table 8-4: Partition coefficients and bioconcentration factors	
Partition coefficient	**Factors**
Solids-water	Chemical class for Koc-QSAR: non-hydrophobic (default QSAR); default non-hydrophobic values have been used, however a better indication of solid-water
Air-water	Henry's law constant: 7.13E-03 pa.m^3.mol^{-1}; Default environmental temperature, solubility and vapour pressure values have been used
Bioconcentration factors	Default bioconcentration factors used for human exposure and predator exposure: Bioconcentration factor for earthworms: 0.848 $l.kgwwt^{-1}$ Bioconcentration factor for fish: 1.41 $l.kgwwt^{-1}$ Bioaccumulation factor for meat: 7.94E-07 Bioaccumulation factor for milk: 7.94E-06
Biota-water	Default bioconcentration factor for aquatic biota used: 1.41 l.kgwwt-^{1}

TFA has been identified as having a low surface tension, a low Log P_{ow}, and has also been shown to have low potential for bioaccumulation in other studies (as shown in the TFA REACH registration dossier) (ECHA 2017d).

Furthermore two studies submitted as part of the REACH registration dossier suggest that:

"TFA-anion poorly adsorbs to the different soil components because after 16 hours of agitating in a soil/water system less than 3% of the initial amount of TFA had disappeared from the water phase. Trifluoroacetate can be considered as a mobile organic compound in soils."

"Concentrations of trifluoroacetate (TFA) in the environment are expected to increase because it is an atmospheric degradation product of CFC replacement compounds that will receive widespread use. TFA possesses high water solubility and its movement in the biosphere will be closely linked with the hydrologic cycle. Surface waters and sediment pore waters will receive loadings directly through precipitation and runoff and indirectly via soil-and ground-water inputs. Studies were conducted to assess whether TFA could be metabolized under aerobic conditions by microbial communities in freshwater surface sediments. Sediment samples were collected to a depth of 2 -3 mm from flowing-water mesocosms in which organisms were pre-exposed to 30 µg TFA/L over a 2.5 year period and from control mesocosms that received no TFA. The sediment-associated microbial communities were tested for ability to incorporate of 2 -[14C]TFA (added at 43 µg/L) in time course experiments. The communities pre-exposed to TFA in the mesocosms showed a low, but statistically significant level of radiolabel incorporation. The cell-specific rate of incorporation for communities sampled from the TFA mesocosms increased nearly 20 -fold during the 2.5 year experiment, from 1.15 x 10^-13 to 2.22 x 10^-12 µg/cell/day. Communities from the control mesocosm never showed statistically significant incorporation. Communities pre-exposed to TFA from 1.5 years also incorporated [14C]TFA when exposed to concentrations as low as 2 µg/L. These results indicate a low level of incorporation of the xenobiotic TFA by natural microbial communities and thus their potential to serve as a point for TFA to enter into the food web."

In the Solvay TFA SDS (Solvay, 2015) the following information on mobility in soil is supplied:

Mobility in soil

Adsorption potential (K_{oc})

TFA is not expected to adsorb on soil (source is unpublished internal reports).

Known distribution to environmental compartments

The Ultimate destination of the product is water.

K_{oc} estimation

Soil adsorption coefficient data was not identified for TFA (although data may be available), however, several models have been developed for calculating K_{oc} and most of these are based on the K_{ow}. Such a model (including models for different chemical classes) has been proposed by Sabljic et al 1995:

$$Koc = \frac{1.26 \cdot Kow^{0.81}}{1000}$$

Using this equation, a low K_{oc} (low sediment adsorption/high sediment to water) is expected.

8.3.3 Degradation and transformation rates

Characterisation of biodegradation

TFA is not biodegradable from the results in VEGA (Section 4.2). For STP (Sewage Treatment Plants), water/sediment, air and soil; the default values in EUSES have been used. Default values were also used for the removal rate constants in soil was used. Using 0 (zero) as a biodegradation end point provides a more precautionary output.

8.3.4 Release estimate

Emission estimates from Section 3 (MIT-5 approach) have been used as the basis for input for this part of the risk assessment along with information from the REACH registration dossier (ECHA, 2017d).

Characterisation and tonnage

TFA is registered under REACH as being manufactured and/or imported into the EEA in the tonnage range of 1,000-10,000 tonnes so is a high production chemical (>1,000 tonnes per annum). For the production volume of the chemical in the EU; 10,000 tonnes per year has been used as the upper tonnage data publically available.

Table 8-5: Characterisation and tonnage information used in the model (2025)	
Required characterisation and tonnage information	**Details**
Fraction of EU production volume for region	100% has been assumed
Regional production volume of substance	10,000 tonnes per year
Continental production volume of substance	10,000 tonnes per year (based on highest REACH tonnage band)
Volume of chemical imported to EU	Assumed 0
Volume of chemical exported from EU	Assumed 0
Tonnage of substance in Europe	10,000 tonnes per year

Table 8-6: Characterisation and tonnage information used in the model (2100 plateau)	
Required characterisation and tonnage information	**Details**
Fraction of EU production volume for region	100% has been assumed
Regional production volume of substance	100,000 tonnes per year
Continental production volume of substance	100,000 tonnes per year (based on increased production)
Volume of chemical imported to EU	Assumed 20,000
Volume of chemical exported from EU	Assumed 0
Tonnage of substance in Europe	120,000 tonnes per year

Table 8-7: Characterisation and tonnage information used in the model (2100 phase-out)	
Required characterisation and tonnage information	**Details**
Fraction of EU production volume for region	100% has been assumed
Regional production volume of substance	10 tonnes per year
Continental production volume of substance	10 tonnes per year (based on reduced production)
Volume of chemical imported to EU	Assumed 0
Volume of chemical exported from EU	Assumed 0
Tonnage of substance in Europe	10 tonnes per year

For the 2100 plateau model, it has been assumed that there will be some importing of TFA. For the 2100 phase-out model, it has been assumed that a small quantity of TFA may still be produced within the EU.

Use patterns for the emission input data

The usage/production title that has been used in the model is HFO/TFA various usage. The main industrial categories that have been used in the model are:

- Category 5: Personal domestic use; and
- Category 6: Public domain

The main use category used in the model is category 29: Heat transferring agents.

As part of further work, the following categories could also be investigated:

- Category 3: Chemical industry-chemicals used in synthesis; and
- Category 15/0: Others- defined as waste recycling operations and other.

Regional and continental total emissions

From the literature review performed in Parts 1 and 2 of the study; emissions of HFO will be emitted to the air with decomposition to TFA in the atmosphere which will reach the ground through precipitation. Using the projected emissions of HFOs presented in Section 3, it has been assumed that the continental levels of emissions will be half of the non-Article 5 countries and regional emissions of the EU will be a third of the continental value. The values have been used as precautionary worst case scenarios.

In the risk assessment, it has also been assumed that 95% of the emissions will be emitted to the air and using the non-Article 5 countries emissions there would also be secondary emissions. In the risk assessment model, this has been assumed to be 0.5% to wastewater, 1.5% to surface water, 1.5% to industrial soil and 1.5% to agricultural soil (within EUSES emission enter different compartments). The emission values used are presented in the following tables.

Table 8-8: Continental HFO-1234yf/TFA total emissions – plateau

Emission	Unit	2025	2050	2075	2100
Total continental emissions to air	kg/per/day	71,475	297,547	302,207	305,282
Total continental emissions to wastewater	kg/per/day	376	1,566	1,591	1,607
Total continental emissions to surface water	kg/per/day	1,129	4,698	4,772	4,820
Total continental emissions to industrial soil	kg/per/day	1,129	4,698	4,772	4,820
Total continental emissions to agricultural soil	kg/per/day	1,129	4,698	4,772	4,820

Table 8-9: Continental HFO-1234yf/TFA total emissions – phase-out

Emission	Unit	2025	2050	2075	2100
Total continental emissions to air	kg/per/day	71,475	297,547	38,783	0
Total continental emissions to wastewater	kg/per/day	376	1,566	204	0
Total continental emissions to surface water	kg/per/day	1,129	4,698	612	0
Total continental emissions to industrial soil	kg/per/day	1,129	4,698	612	0
Total continental emissions to agricultural soil	kg/per/day	1,129	4,698	612	0

Table 8-10: Regional HFO-1234yf/TFA total emissions – plateau

Emission	Unit	2025	2050	2075	2100
Total continental emissions to air	kg/per/day	23,825	99,182	100,736	101,761
Total continental emissions to wastewater	kg/per/day	125	522	530	536
Total continental emissions to surface water	kg/per/day	376	1,566	1,591	1,607
Total continental emissions to industrial soil	kg/per/day	376	1,566	1,591	1,607
Total continental emissions to agricultural soil	kg/per/day	376	1,566	1,591	1,607

Table 8-11: Regional HFO-1234yf/TFA total emissions – phase-out

Emission	Unit	2025	2050	2075	2100
Total continental emissions to air	kg/per/day	23,825	99,182	12,928	0
Total continental emissions to wastewater	kg/per/day	125	522	68	0
Total continental emissions to surface water	kg/per/day	376	1,566	204	0
Total continental emissions to industrial soil	kg/per/day	376	1,566	204	0
Total continental emissions to agricultural soil	kg/per/day	376	1,566	204	0

Local emissions

For an episode release in 2025, the worst case assumption has been used. This assumption involves 10,000 tonnes (highest REACH registration tonnage) being produced in the EU. For the number of plants manufacturing HFOs, three plants have been assumed (there is limited information on manufacturing) and it has been assumed that each plant would manufacture the same volume of HFOs and would manufacture HFOs for 225 days a year. Also, it has been assumed that 50% of an entire day's production is emitted to air as part of an episode, 7,407 kg/day with zero emissions to waste water. This has also been modified for 2100 plateau and 2100 phase-out.

8.3.5 Regional, continental and global distribution

For distribution, published values have been used, in particular, the Switzerland river waters levels. The data points in a variety of media require further investigation.

Table 8-12: Regional, contribution and global distribution

Distribution	Geographical information	Values used
Rainwater and snow	Switzerland	3-1,550 ng a.e./L; 0.000328 mg/L
	Chile, Malawi and Canada	6-87, 4-15, and <0.5-350 ng a.e./L, respectively
	Japan	29-76 ng a.e./L
	Guangzhou, China	46-974 ng a.e./L
Soils	Canada	<0.0-1,400 ng a.e./kg dry weight (d.w.)
	Malawi	<100-7,500 ng a.e./kg d.w.
	UK	850-5,000 ng a.e./kg d.w. 0.005 mg used for all sediments, including marine
	Chile	100–9,400 ng a.e./kg d.w.
Surface waters (rivers, lakes, wetlands)	Germany	540-140000 ng a.e./L *used for fresh water
	Switzerland	Rivers = 12-328 Midland lakes = 37-204 Mountain lakes = 46-360 Moor water = 59-175 Drinking water = 16-123 (values in ng a.e./L)
Oceans	-	200 ng a.e./L is considered to be a representative value
a.e= acid equivalents		

Local concentrations and depositions

Automatic calculations in EUSES were used.

Local PECs (production)

Automatic calculations in EUSES were used.

8.3.6 Exposure

Secondary poisoning

There is no readily available information in the literature on the secondary poisoning and concentrations in fish and earthworms.

8.3.7 Human exposed to or via the environment

Regional and local concentration in wet fish, meat and milk

Information about regional concentrations in wet fish, root tissue of plant, leaves of plant and in grass is not readily available (Rollins et al, 1989).

However, drinking water concentrations have been identified as being (the upper Switzerland value was used, more information is provided in section 6.2.1):

Table 8-13: Drinking water

Location	Concentration (ng a.e./L)
Switzerland	16-123
Beijing	155

Meat, milk and cattle intake information has not yet been identified; however, default model values have been calculated.

8.3.8 Microorganisms in a STP

The values in the table below were generated in accordance with OECD 209 Guidelines and measured the influence of sodium trifluoroacetate on activated sludge.

Table 8-14: Microorganisms in a STP

Parameter	Concentration (mg/L)
EC_{50}	> 832
EC_{10}	> 832
NOEC	> 832

8.3.9 Aquatic organisms

Freshwater

The table overleaf describes the LC_{50} and NOEC values for three freshwater aquatic organisms which have been used for the risk assessment.

Table 8-15: Freshwater aquatic organisms	
Species	**LC_{50} / NOEC concentration (mg/L)**
Zebrafish (*Danio rerio*) (fish)	>1,200 mg/L/ 1,200 mg NaTFA salt/L
Water fleas (*Daphnia magna*) (crustacean)	>1,200 mg/L (EC_{50}) / 1,200 mg NaTFA salt/L
Pseudokirchneriella subcapitata (algae)*	0.62 mg/L (EC_{50}) TFA[#]
Note:*Known as *Raphidocelis subcapitata* and *Selenastrum capricornutum* also	

However, there is some uncertainty surrounding the freshwater algae data in the table above. In the conclusion of the REACH registration dossier (ECHA, 2017d) it was indicated that due to the low number of replicates, EC_{50} for 72h values could only be considered as rough estimates. Solomon (Solomon et al 2016) also suggested that the alga species used in the test was unusually sensitive and that retesting is needed.

All fresh water and marine algae data from the ECHA REACH registration dossier is indicated in the table below.

Table 8-16: Algae toxicity				
Type of information	**Water**	**Species**	**EC_{50} / NOEC concentration (mg/L)**	**Klimisch reliability level**
Read-across (sodium trifluoroacetate)	Fresh water	*Pseudokirchneriella subcapitata*	0.74 (EC_{50}) (NaTFA) / 0.62 (EC_{50}) (TFA)*	2
Read-across (sodium trifluoroacetate)	Fresh water	*Pseudokirchneriella subcapitata*	1.2 (EC_{50}) (TFA)	2
Read-across (sodium trifluoroacetate)	Fresh water	*Desmodesmus subspicatus*	>99.9 (EC_{50}) (TFA)	2
Read-across (sodium trifluoroacetate)	Fresh water	*Chlorella vulgaris*	>999 (EC_{50}) (TFA) 999 (NOEC) (TFA)	1
Read-across (sodium trifluoroacetate)	Fresh water	*Chlamydomonas reinhardtii*	>99 (EC_{50}) (TFA) 99 (NOEC) (TFA)	1
Read-across (sodium trifluoroacetate)	Marine water	*Dunaliella tertiolecta*	103 (EC_{50}) (TFA) <103 (NOEC) (TFA)	1
Read-across (sodium trifluoroacetate)	Marine water	*Phaeodactylum tricornutum*	>97 (EC_{50}) (TFA) 97 (NOEC) (TFA)**	1
Read-across (sodium trifluoroacetate)	Fresh water	*Microcystis aeruginosa*	>97 (EC_{50}) (TFA) 97 (NOEC) (TFA)**	2
Read-across (sodium trifluoroacetate)	Fresh water	*Navicula pelliculosa*	999 (EC_{50}) (TFA) (biomass) 1,997 (EC_{50}) (TFA) (growth rate) 499 (NOEC) (TFA) 499 (NOEC) (TFA)	2
Read-across (sodium trifluoroacetate)	Marine water	*Skeletonema costatum*	1,997 (EC_{50}) (TFA) 1,997 (NOEC) (TFA)	1

Read-across (sodium trifluoroacetate)	Fresh water	*Anabaena flos-aquae*	1,997 (EC_{50}) (TFA) (120 h) 499 (NOEC) (TFA) (120 h)	1
Read-across (sodium trifluoroacetate)	Fresh water	*Pseudokirchneriella subcapitata*	0.3 (LOEC) (TFA)*** 0.1 (NOEC) (TFA)	2
Read-across (sodium trifluoroacetate)	Fresh water	*Pseudokirchneriella subcapitata*	No EC_{50}, NOEC or LOEC calculated	2
Read-across (sodium trifluoroacetate)	Fresh water	*Pseudokirchneriella subcapitata*	1.2 (EC_{50}) (TFA) **** 0.25 (NOEC) (TFA)	2
Read-across (sodium trifluoroacetate)	Fresh water	*Pseudokirchneriella subcapitata*	120 (EC_{50}) (TFA-Na) 1,200 (EC_{20}) (TFA-Na)	2
Read-across (sodium trifluoroacetate)	Fresh water	*Pseudokirchneriella subcapitata*	Biocentration: The final conclusions are that the radioactive labelled TFA was accumulated around ten times by the algal cells from the media ; no more than 2 - 4 % conversion of TFA to DFA or MFA did occurred.	2
TFA	Fresh water	*Pseudokirchneriella subcapitata*	24.7 (EC_{50}) (TFA) (biomass) 145 (EC_{50}))TFA) (growth rate) 6 (NOEC) (TFA)	4

*Due to the low number of replicates, EC_{50} for 72h values can only be considered as rough estimates

**Limit test, not toxicity at the maximum range

***A study was realised in agreement with OECD Guideline 201 with deviations. The validity criteria were all fulfilled. However the highest concentration tested resulted in an inhibition of only 6% of the growth rate which doesn't allow to derive an EC_{50} value

****Not GLP and some important information is missing on the test parameter

As indicated, some of the endpoints were based on limit tests and within these tests an EC_{50} was not determined and the result was indicated as being a greater than expected value. The only algae species to record a result of <10 mg/L was *Pseudokirchneriella subcapitata*. In one of the *Pseudokirchneriella subcapitata* studies the highest inhibition of growth recorded was only 6%. Some of the studies also appear to be limit tests and a greater than expected result has been indicated. For these tests the EC_{50} concentration is likely to be higher than the result indicated.

As these toxicity values vary significantly and that these would have a significant outcome on the model, a range of EC_{50} values have been used in the model. The values that have been used are the most toxic fresh water and marine water algae results, the median results and the average result (limit tests and greater than results were used when determining the average and median values). A summary of the values is presented in the table overleaf.

Table 8-17: Fresh water toxicity to algae (mg/L)				
Endpoint	Most toxic	Average value (range)	Median	Least toxic
EC_{50}	0.62	441 (0.62 – 1997)	99	1997
NOEC	0.1	275 (0.1 – 999)	98	999

Marine water

Table 8-18: Marine water toxicity to algae (mg/L)				
Endpoint	Most toxic	Average value (range)	Median	Least toxic
EC_{50}	>97	732 (97 – 1997)	103	1997
NOEC	97	732 (97 – 1997)	103	1997

No other marine water data was given in the REACH registration dossier and there is a lack of available information in other literature.

Freshwater sediment

No data was given in the REACH registration dossier and there is a lack of available information in other literature.

Freshwater sediment

No data was given in the REACH registration dossier and there is a lack of available information in other literature.

8.3.10 Terrestrial

An EC_{50} for terrestrial plants has been established (presented below).

Table 8-19: Terrestrial plants	
Species	EC_{50} concentration (mg NaTFA/kg)
Plants	250 mg NaTFA/kg

There is no other terrestrial data or long term NOEC studies listed in the REACH registration dossier.

8.3.11 Birds

No toxicity tests have been published for birds.

8.3.12 Mammals

Repeated dose

The oral NOAEL has been established using a rat test species with the value given overleaf.

Table 8-20: Repeated dose oral NOAEL	
Species	**Oral NOAEL (mg/g bw/day)**
Rat (Sprague-Dawley)	1,000

There is a lack of available information with the LOAEL and CED values not available in the REACH registration dossier. No dermal data is available in the registration dossier and no inhalatory LOAEL has been assigned due to it having a Klimisch score of Level 4.

Fertility

The fertility oral NOAEL has been established using a rat test species with the value given below.

Table 8-21: Fertility oral NOAEL	
Species	**Oral NOAEL (mg/g bw/day)**
Rat	1,000

Maternal-tox

The maternal toxicity oral NOAEL has been established using a rat test species with the value given below.

Table 8-22: Maternal toxicity oral NOAEL	
Species	**Oral NOAEL (mg/g bw/day)**
Rat	150

Development-tox

The development toxicity oral NOAEL has been established using a rat test species with the value given below.

Table 8-23: Development toxicity oral NOAEL	
Species	**Oral NOAEL (mg/g bw/day)**
Rat	150

Carc (threshold)

There is no information available on the REACH registration dossier.

Carc (non-threshold)

There is no information available on the REACH registration dossier.

Acute

No value was assigned for acute toxicity due to it having a Klimisch score of Level 4 (the LC_{50} was 10 mg/L in rats, in a 2 hour exposure test).

Predator

There is no information available on the REACH registration dossier.

Bio-availability

There is no information available on the REACH registration dossier.

8.3.13 Humans

No human data is publically available for the following aspects (however, some mammalian data is available and has been indicated in 8.3.12 Mammals):

- Repeated dose;
- Fertility;
- Maternal toxicity;
- Development toxicity;
- Carcinogenicity (threshold); and
- Bioavailability.

8.3.14 Environmental effects assessment

The pre-populated data in EUSES has not been amended for the environmental effects assessment. Data from ECHA REACH registration dossier (ECHA, 2017d) data has been used for the following:

- The STP data has been used (STP (PNEC STP): 83.2 mg/L; Assessment factor: 10);
- The PNEC sediment data (fresh) has been used (Sediment (freshwater PNEC sediment): 4.22 mg/kg sediment dw); and
- The PNEC sediment data (marine) has been used (Sediment (marine water PNEC sediment): 0.422 mg/kg sediment dw).

8.3.15 Risk characterisation

Additional data is required to produce a risk characterisation.

8.4 EUSES assessment results

Preliminary results for the risk assessment for HFO refrigerants for the following scenarios have been obtained for the following:

- For 2025 (highest algae toxicity data);
- For 2100 plateau in HFOs from 2050 (highest algae toxicity data);
- For 2100 phase-out of HFOs in 2050 (highest algae toxicity data);
- For 2025 (median algae toxicity data);
- For 2100 plateau in HFOs from 2050 (median algae toxicity data);
- For 2100 phase-out of HFOs in 2050 (median algae toxicity data);
- For 2025 (average algae toxicity data);
- For 2100 plateau in HFOs from 2050 (average algae toxicity data); and
- For 2100 phase-out of HFOs in 2050 (average algae toxicity data).

The 2025 data is predicted to be the same for both the 2025 plateau and 2025 phase-out scenarios. This data and the emissions data for 2100 plateau and 2100 phase-out is based on the emissions data for non-A5 countries which is discussed in Section 4 (Table 4-2).

The emission assumptions for the EU used are based on 50% of non-A5 country emissions. The model outputs for the 2100 plateau and 2100 phase-out scenarios are presented the Annex.

The model outputs include Risk Characterisation Ratios (RCR) and Margin of Safety (MOS) information. The RCR is the ratio of Predicted Environmental Concentration (PEC) to Predicted No-Effect Concentration (PNEC), this is calculated for environmental compartments (fresh water, marine, fresh-water sediment, marine sediment, soil, sewage treatment plants (STP)) and species (marine fish, marine top-predators and worms). An RCR of >1 equates to a risk.

For the human end-point, the MOS is the ratio of the estimated no-effect or effect level parameter to the estimated exposure level for human sub-populations. MOS values have been calculated based upon the available endpoints for TFA; these are repeated dose toxicity (inhalation) repeated dose toxicity (total), fertility (inhalation), fertility (total), maternal toxicity (inhalation), maternal toxicity (total), developmental toxicity (inhalation) and developmental toxicity (total). Carcinogenicity, non-threshold and lifetime cancer risk have not been calculated due to a lack of carcinogenicity data. However, the VEGA QSAR data, calculated based on substances with a similar chemicals structure, suggests that that substance is not expected to be carcinogenic (however further QSAR data or laboratory studies could be conducted). A low MOS equates to a risk, a MOS value of at least 100 is generally considered to be protective.

RCR and MOS values that equate to a risk are highlighted using red text. The source of the RCR and MOS is shown by the usage/step.

8.4.1 Assessment for 2025 (same in plateau and phase-out)

For 2025, as shown in Tables 8-24 to Table 8-26, there is expected to be a risk developing in a number of compartments from the emissions of TFA from a number of sources.

The highest RCR values calculated appear to be for soil, however it is anticipated that these have been overestimated, perhaps by orders of magnitude. The reason for this is that most emission has been assumed to be emitted to the air and TFA is assumed to be deposited into various environmental compartments, with one of the biggest being soils (urban, agricultural and natural). Although TFA is predicted to be mobile, it is unknown how volatile it is and the model assumes that this will be limited. Therefore, due to high levels of atmosphere emissions and volumes entering soils (one of the main initial compartments TFA enters) the risk here is assumed to be higher compared to other compartments. Also, as indicated previously, toxicity to plants and microorganisms is higher in than it is in some aquatic species.

Table 8-24: Risk characterisation result for the environment, assessment for 2025 (highest algae toxicity data)

Usage/step	Fresh water	Marine	Fr. sed.	Mar. sed.	Soil	STP	Fish	Mar. fish	Mar. top	Worm
Chemical production	1.28	15.5	12.8	15.5	6.81 E+03	9.14 E-03	1.2 E-04	1.91 E-05	1.06 E-05	0.0491
Personal/ domestic	13.8	16.5	13.8	16.5	61.4	9.85 E-03	1.88 E-03	2.58 E-05	1.2 E-05	4.52 E-04
Light industrial use	52.3	55	52.3	55	63	0.0386	1.07 E-04	1.78 E-05	1.03 E-05	4.6 E-04
Regional	0.529	3.23	10	100	59.6					

Fr. sed. = Fresh water sediment; Mar. Sed. = Marine sediment; Mar. fish = Marine fish, Mar. top = Marine top predator

Table 8-25: Risk characterisation result for the environment, assessment for 2025 (median algae toxicity data)										
Usage/step	Fresh water	Marine	Fr. sed.	Mar. sed.	Soil	STP	Fish	Mar. fish	Mar. top	Worm
Chemical production	8.01 E-03	0.097	0.0801	0.097	42.6	9.14 E-03	1.2 E-04	1.91 E-05	1.06 E-05	0.0491
Personal/ domestic	0.0861	0.103	0.0861	0.103	0.384	9.85 E-03	1.88 E-03	2.58 E-05	1.2 E-05	4.52 E-04
Light industrial use	0.328	0.345	0.328	0.345	0.395	0.0386	1.07 E-04	1.78 E-05	1.03 E-05	4.6 E-04
Regional	3.31 E-03	0.0202	0.0628	0.628	0.373					
Fr. sed. = Fresh water sediment; Mar. Sed. = Marine sediment; Mar. fish = Marine fish, Mar. top = Marine top predator										

Table 8-26: Risk characterisation result for the environment, assessment for 2025 (average algae toxicity data)										
Usage/step	Fresh water	Marine	Fr. sed.	Mar. sed.	Soil	STP	Fish	Mar. fish	Mar. top	Worm
Chemical production	1.8 E-03	0.0218	0.018	0.0218	9.57	9.14 E-03	1.2 E-04	1.91 E-05	1.06 E-05	0.0491
Personal/ domestic	0.0193	0.0231	0.0193	0.0231	0.0863	9.85 E-03	1.88 E-03	2.58 E-05	1.2 E-05	4.52 E-04
Light industrial use	0.0736	0.0774	0.0736	0.0774	0.0886	0.038 6	1.07 E-04	1.78 E-05	1.03 E-05	4.6 E-04
Regional	7.44 E-04	4.54 E-03	0.0141	0.141	0.0838					
Fr. sed. = Fresh water sediment; Mar. Sed. = Marine sediment; Mar. fish = Marine fish, Mar. top = Marine top predator										

The algae toxicity has an impact on the RCR of all the environmental compartments; however the risk to fish, marine fish, marine top predators and worms appears to be low.

There also appears to be a risk to most of the environmental compartments, with light industrial use being a particular contributor. Assuming that there are emissions/releases to the environment from production facilities, this is where the risk is likely to be the highest, and the largest risk could possibly be to fresh water fish.

As shown in Table 8-27, in 2025, the MOS is greater than 100 for all toxicological endpoints, the lowest MOS was identified for maternal toxicity (total) and development toxicity (total).

Table 8-27: Margin of Safety (MOS) for humans exposed to or via the environment, assessment for 2025								
Usage/step	Repdose	Repdose	Fert.	Fert.	Mater.	Mater.	Devel.	Devel.
	Inh.	Total	Inh.	Total	Inh.	Total	Inh.	Total
Chemical production	7.55 E+10	6.32 E+03	7.55 E+10	6.32 E+03	1.13 E+10	947	1.13 E+10	947
Personal/ domestic	6.29 E+06	2.27 E+05	6.29 E+06	2.27 E+05	9.44 E+05	3.4 E+04	9.44 E+05	3.4 E+04
Light industrial use	4.6 E+06	1.81 E+05	4.6 E+06	1.81 E+05	6.89 E+05	2.72 E+04	6.89 E+05	2.72 E+04
Regional	4.27 E+11	1.38 E+08	4.27 E+11	1.38 E+08	6.4 E+10	2.07 E+07	6.4 E+10	2.07 E+07
Note: Carcinogenic threshold, non-threshold and CLR is not applicable Repdose = Repeat dose toxicity; Fert = Fertility toxicity; Mater. = Maternal toxicity; Devel. = Developmental toxicity; Inh. = Inhalation								

8.4.2 2100 plateau

For the 2100 plateau, as shown in Tables 8-28 to 8-30, there is expected to be a risk developing in a number of compartments from the emissions of TFA from a number of sources. The most significant changes between 2025 and 2100 plateau are the increasing risk from all uses, in particularly light industrial use sources. However, despite significant increases of TFA in the environment, the RCR calculated for species suggests that in the environment there is limited risk to species, with the biggest risk being to fresh water fish and worms close to production facilities.

Table 8-28: Risk characterisation result for the environment, assessment for 2100 plateau (highest algae toxicity data)										
Usage/step	Fresh water	Marine	Fr. sed.	Mar. sed.	Soil	STP	Fish	Mar. fish	Mar. top	Worm
Chemical production	1.21 E+03	121 E+04	1.21 E+04	1.21 E+04	1.73 E+04	9.01	0.0131	0.0131	2.62 E-03	0.123
Personal/ domestic	1.82 E+04	1.82 E+04	1.82 E+04	1.82 E+04	590	13.6	0.24	0.024	4.8 E-03	2.26 E-03
Light industrial use	3.85 E+04	3.85 E+04	3.85 E+04	3.85 E+04	1.18 E+03	28.7	0.0693	6.94 E-03	1.4 E-03	4.27 E-03
Regional	0.529	3.23	10	100	59.6					
Fr. sed. = Fresh water sediment; Mar. Sed. = Marine sediment; Mar. fish = Marine fish, Mar. top = Marine top predator										

Table 8-29: Risk characterisation result for the environment, assessment for 2100 plateau (median algae toxicity data)										
Usage/step	Fresh water	Marine	Fr. sed.	Mar. sed.	Soil	STP	Fish	Mar. fish	Mar. top	Worm
Chemical production	7.57	75.8	75.7	75.8	108	9.01	0.0131	0.0131	2.62 E-03	0.123
Personal/ domestic	114	114	114	114	3.7	13.6	0.24	0.024	4.8 E-03	2.26 E-03
Light industrial use	241	241	241	241	7.37	28.7	0.0693	6.94 E-03	1.4 E-03	4.27 E-03
Regional	3.31 E-03	0.0202	0.0628	0.628	0.373					
Fr. sed. = Fresh water sediment; Mar. Sed. = Marine sediment; Mar. fish = Marine fish, Mar. top = Marine top predator										

Table 8-30: Risk characterisation result for the environment, assessment for 2100 plateau (average algae toxicity data)										
Usage/step	Fresh water	Marine	Fr. sed.	Mar. sed.	Soil	STP	Fish	Mar. fish	Mar. top	Worm
Chemical production	1.7	17	17	24.3	9.01	9.01	0.0131	0.0131	2.62 E-03	0.123
Personal/ domestic	25.6	25.7	25.6	25.7	0.83	13.6	0.24	0.024	4.8 E-03	2.26 E-03
Light industrial use	54.2	54.2	54.2	1.66	28.7	28.7	0.0693	6.94 E-03	1.4 E-03	4.27 E-03
Regional	7.44 E-04	4.54 E-03	0.0141	0.141	0.0838					
Fr. sed. = Fresh water sediment; Mar. Sed. = Marine sediment; Mar. fish = Marine fish, Mar. top = Marine top predator										

As shown in Table 8-31, in 2100 plateau, although a number of MOS have decreased by an order of magnitude, all MOS are greater than 100 for all toxicological endpoints. The lowest MOS was identified for maternal toxicity (total) and development toxicity (total), and in particular the biggest risk might be close to production facilities and from personal/domestic use.

Table 8-31: Margin of Safety (MOS) for humans exposed to or via the environment, 2100 Plateau								
Usage/step	Repdose	Repdose	Fert.	Fert.	Mater.	Mater.	Devel.	Devel.
	Inh.	Total	Inh.	Total	Inh.	Total	Inh.	Total
Chemical production	6.26 E+10	2.43 E+03	6.26 E+10	2.43 E+03	9.4 E+09	364	9.4 E+09	364
Personal/domestic	3.15 E+06	2.8 E+03	3.15 E+06	2.8 E+03	4.72 E+05	420	4.72 E+05	420
Light industrial use	3.06 E+06	9.05 E+03	3.06 E+06	9.05 E+03	4.6 E+05	1.36 E+03	4.6 E+05	1.36 E+03
Regional	4.27 E+11	1.38 E+08	4.27 E+11	1..8 E+08	6.4 E+10	2.07 E+07	6.4 E+10	2.07 E+07
Note: Carcinogenic threshold, non-threshold and CLR is not applicable Repdose = Repeat dose toxicity; Fert = Fertility toxicity; Mater. = Maternal toxicity; Devel. = Developmental toxicity; Inh. = Inhalation								

8.4.3 2100 phase-out

In 2100 phase-out, very small levels of TFA production and emissions are still assumed to occur, however as shown in Tables 8-33 and 8-34 (median and average algae toxicity data), in 2100 phase-out, there is not expected to be a risk as no RCR is greater than 1. Due to the persistence of TFA, there will still be levels of TFA present in the environment. However, these levels are not expected to pose a risk to species.

Table 8-32: Risk characterisation result for the environment, assessment for 2100 phase-out (median algae toxicity data)										
Usage/step	Fresh water	Marine	Fr. sed.	Mar. sed.	Soil	STP	Fish	Mar. fish	Mar. top	Worm
Chemical production	0.0508	0.525	0.508	0.525	0.424	0.0601	8.84 E-04	9.55 E-05	2.59 E-05	4.9 E-04
Personal/ domestic	0.0116	0.0285	0.0116	0.0285	0.378	9.85 E-04	3.13 E-05	1.02 E-05	8.82 E-06	4.46 E-04
Light industrial use	0.256	0.273	0.273	0.273	0.383	0.03	8.64 E-05	1.57 E-05	9.93 E-06	4.48 E-04
Regional	3.31 E-03	0.0202	0.0202	0.628	0.373					
Fr. sed. = Fresh water sediment; Mar. Sed. = Marine sediment; Mar. fish = Marine fish, Mar. top = Marine top predator										

Table 8-33: Risk characterisation result for the environment, assessment for 2100 phase-out (average algae toxicity data)										
Usage/step	Fresh water	Marine	Fr. sed.	Mar. sed.	Soil	STP	Fish	Mar. fish	Mar. top	Worm
Chemical production	0.0114	0.118	0.114	0.118	0.0951	0.060 1	8.84 E-04	9.55 E-05	2.59 E-05	4.9 E-04
Personal/ domestic	2.6 E-03	6.39 E-03	2.6 E-03	6.39 E-03	0.848	9.85 E-04	3.13 E-05	1.02 E-05	8.82 E-06	4.46 E-04
Light industrial use	0.0574	0.0612	0.0574	0.0612	0.086	0.03	8.64 E-05	1.57 E-05	9.93 E-06	4.48 E-04
Regional	7.44 E-04	4.54 E-03	0.0141	0.141	0.0838					
Fr. sed. = Fresh water sediment; Mar. Sed. = Marine sediment; Mar. fish = Marine fish, Mar. top = Marine top predator										

As shown in Table 8-34, in 2100 phase-out, the MOS is large for all toxicological endpoints and all endpoints are greater than 100. The lowest MOS still exist for both maternal toxicity (total) and development toxicity (total).

Table 8-34: Margin of Safety (MOS) for humans exposed to or via the environment, 2100 phase-out								
Usage/step	Repdose Inh.	Repdose Total	Fert. Inh.	Fert. Total	Mater. Inh.	Mater. Total	Devel. Inh.	Devel. Total
Chemical production	6.26 E+10	6.57 E+06	6.26 E+10	6.57 E+05	9.4 E+09	9.85 E+04	9.4 E+09	9.85 E+05
Personal/ domestic	1.26 E+07	4.51 E+05	1.26 E+07	4.51 E+05	1.89 E+06	6.76 E+04	1.89 E+06	6.76 E+04
Light industrial use	2.3 E+07	6.13 E+05	2.3 E+07	6.13 E+05	3.45 E+06	9.19 E+04	3.45 E+06	9.19 E+04
Regional	4.27 E+11	1.38 E+08	4.27 E+11	1.38 E+08	6.4 E+10	2.07 E+07	6.4 E+10	2.07 E+07
Note: Carcinogenic threshold, non-threshold and CLR is not applicable Repdose = Repeat dose toxicity; Fert = Fertility toxicity; Mater. = Maternal toxicity; Devel. = Developmental toxicity; Inh. = Inhalation								

8.4.4 Discussion

Risk to the environment

TFA, as previously identified is not expected to be bioaccumulative and has not been shown to exhibit toxicological properties of concern. However, the substance is very persistent and concentrations of TFA will only be expected to increase. In the 2100 plateau, this might be particularly concerning as the precipitation is likely to cause a significant increase in levels of TFA not only in the expected final compartment (the aquatic environment) but also those compartments which TFA enters (soils) on its way to entering its final compartment. TFA has also been shown to cause some toxicity to plants and soil organisms. There are also some data points that are currently missing due to a lack of available information and these are discussed in Section 8.5.

Risk to humans

The margin of safety for human health is reduced in 2100 for the plateau of HFO emissions from 2025. Therefore, phasing out HFOs (and therefore TFA) or using emission reduction strategies along with using best practise measures that help ensure efficient capturing of HFO/TFA during recycling operations will help to reduce the risk to human and environmental health. The largest risk to human health is likely to be close to areas of production facilities and urban areas where it is used in devices for personal and domestic use.

For some data points, there is a lack of information and these are discussed in Section 8.5.

Comparison with other risk assessments

Solomon et al (2016) compared the risks of TFA in various environments based on a comparison of exposure values and toxicity values. The toxicity values used were the most sensitive NOECs, a margin of exposure (MoE), and the ratio of the exposure concentration to the toxicity study was also calculated. It is concluded that there are *de minimis* risks from TFA for humans and terrestrial vertebrates, furthermore as the MoEs are extremely large, and even if exposures increase in the near future, these risks would likely still be *de minimis*. It is also noted that although the risks to humans and environment from the current (and near future) amounts of TFA in the environment are judged to be *de minimis*, TFA is persistent and concentrations continue to increase in terminal sinks.

Boutonnet et al (1999) evaluated the toxicity in stream mesocosms, algae, higher plants, fish, animals and humans. The findings support the idea that there is very low toxicity in all of these systems and that the effect of TFA on seed germination and plant growth has been evaluated in a variety of plants, and concentrations tested did not affect germination or growth.

Furthermore, the European Food Safety Association (EFSA) have provided an opinion for the setting of Maximum Residue Levels (MRL) of TFA in various crops (EFSA, 2014). TFA is a metabolite of a plant protection product. The EFSA study considered dietary exposure from other sources including HFCs. EFSA highlight how Christoph (2002) indicates the highest concentrations of TFA were found in sites close to industrial locations. EFSA concluded that the exposure of the plant protection product saflufenacil and its metabolite TFA via the diet will not result in consumer exposure exceeding the toxicological reference values derived for the parent compound saflufenacil and its metabolite, and is therefore is unlikely to pose a public health concern.

Our environment risk assessment supports this view, the risk to environmental organisms (based on the studies that are available) and human health appears to be low. However, concentrations in the environment will only increase; in particular this is anticipated to occur in terminal sinks. Based on a considerable increase in the emission of HFO/TFA, under the 2100 plateau assumption, the concentrations of TFA entering the environment may increase significantly. The risk under this assumption would therefore increase. The risk to aquatic organisms in 2100 (and other organisms) may also increase due to changes in the climate, sea/ocean temperatures, increased acidity, decreased dissolved oxygen and other factors (Brierley et al, 2009).

Alternative software

The ECHA document, *Guidance on information requirements and Chemical Safety Assessment: Chapter R.16: Environmental exposure assessment* (ECHA, 2016), sets out software for the modelling of environmental risk.

EUSES is indicated as being a decision-support system for the evaluation of the risks of substances to humans and the environment. Also, the system is based on the EU Technical Guidance Documents (TGDs; EC-TGD, 2003) for the risk assessment of new and existing substances and biocides and the EUSES software package as implemented in the ECHA Chesar tool. The ECHA document outlines the use of EUSES and the modelling parameters.

Alternatives to EUSES for performing risk assessments include:

- Chesar 3.3 (ECETOC's Targeted Risk Assessment (TRA)) tool that calculates the risk of exposure from chemicals to workers, consumers and the environment is included within Chesar 3.3;
- USEtox®2.0 which is a scientific consensus model endorsed by the UNEP/SETAC Life Cycle Initiative for characterizing human and ecotoxicological impacts of chemicals. The main output is a database of recommended and interim characterisation factors including fate, exposure, and effect parameters;
- FOCUS which is a model designed for pesticides. However the model could be used to predict the fate of TFA in soils. In EUSES the RCR of TFA in soil was an calculated to be >1;
- CHARM. This model is for use in the offshore oil and gas sector where there are deliberate (permitted) localised discharges of chemicals from oil and gas production operations to the marine environment, although this model could be used some additional sediment data would be required for sediment toxicity. The standard conditions for discharge in CHARM are based on a single point of discharge in standard waters, deep water for oil and shallower waters for gas operations, although if these are modified the output may become unreliable;
- DREAM (Dose related Risk and Effect Assessment Model (DREAM). This software is used in the offshore oil and gas sector and able to account for releases of complex mixtures of

chemicals, i.e. such as those associated with produced water and drilling discharges, the model is again based on discharges specific to offshore oil and gas operations; and
- US EPA models. The US EPA has a range of models, risk tools and databases)

Basic PEC:PNEC calculation

A basic PEC:PNEC approach is highlighted below.

Table 8-35: PNEC calculation for TFA			
Compartment	**Ecotoxicology dose descriptors**	**Assessment factor**	**PNEC value (mg/L)**
PNEC-*Fresh water (most toxic algae)*	*Danio rerio* >1,200 mg/L *Daphnia magna* >1,200 mg/l *Pseudokirchneriella subcapitata* **0.62** mg/L	10 100	0.062 **0.0062**
PNEC-*Fresh water (median toxic algae)*	*Danio rerio* >1,200 mg/L *Daphnia magna* >1,200 mg/L Algae **99** mg/L	10 100	9.9 0.99
PNEC-*Fresh water (average toxic algae)*	*Danio rerio* >1,200 mg/L *Daphnia magna* >1,200 mg/L Algae **441** mg/L	10 100	44.1 4.41
PNEC-*Marine water*	*Phaeodactylum tricornutum* >**97** mg/L	1000	0.097
PNEC-*STP microorganism*	>**832** mg/L	1000	0.832
PNEC-*soil*	-	-	-
PNEC-*plants*	*Phaseolus aureus* >**250** mg/L	1000	0.25

The lowest PNEC value is 0.0062 mg/L.

Table 8-36: Regional, contribution and global distribution, use as Predicted Environmental Concentration (PEC)			
Distribution	**Geographical information**	**Values**	**Highest value (mg/L)**
Rainwater and snow	Switzerland	**3**-1,550 ng a.e./L; 0.000328 mg/L	0.000328
	Chile, Malawi and Canada	6-87, 4-15, and <**0.5**-350 ng a.e./L, respectively	0.00035
	Japan	29-76 ng a.e./L	0.000076
	Guangzhou, China	46-974 ng a.e./L	0.000974
Soils	Canada	<0.0-1,400 ng a.e./kg dry weight (d.w.)	0.0014
	Malawi	<100-7,500 ng a.e./kg d.w.	**0.0075**
	UK	850-5,000 ng a.e./kg d.w. 0.005 mg used for all	0.005

		sediments, including marine	
	Chile	100–9,400 ng a.e./kg d.w.	**0.0094**
Surface waters (rivers, lakes, wetlands)	Germany	540-140000 ng a.e./L *used for fresh water	**0.14**
	Switzerland	Rivers = 12-328 Midland lakes = 37-204 Mountain lakes = 46-360 Moor water = 59-175 Drinking water = 16-123 (ng a.e.L)	0.00036
Oceans	-	200 ng a.e./L is considered to be a representative value	0.0002
a.e= acid equivalents			

Table 8-37: Drinking water		
Location	**Concentration (ng a.e./L)**	**Concentration (mg a.e./L)**
Switzerland	16-123	0.000123
Beijing	155	0.000155

The upper environmental concentrations (PEC) identified in the soils of Malawi and Chile and the surface waters of Germany were equivalent to 0.0075, 0.0094 and 0.14 mg/L a.e. These levels would be greater than the freshwater PNEC of 0.0062 (but not a soil PNEC as one has not been calculated based on a data gap) and would equate to their being an environmental risk. The freshwater PNEC of 0.0062 is based on the most toxic algae study although, the other less toxic (median and average) study data gives a PNEC higher than the upper PEC.

As TFA has been shown to be non-biodegradable, it is anticipated to be a substance that will continue to build up in the environment as more TFA is emitted to the environment. Therefore, the risk to the environment may only increase in the future; the risk will increase if emissions of TFA increase in the future.

8.5 Identified data gaps

A number of data gaps/additional considerations have been identified for TFA in the risk assessment. These are:

- LC_{50} and NOEC for earthworms;
- EC_{50} and NOEC for soil microorganisms;
- LC_{50} and NOEC for other terrestrial species;
- LC_{50}, EC_{10} and NOEC for marine sediment organisms;
- LC_{50}, EC_{10} and NOEC for fresh-water sediment organisms;
- LC_{50} and NOEC for fish (marine);
- $L(E)C_{50}$ and NOEC for crustaceans (marine);
- EC_{50} and NOEC for algae (marine);
- NOEC for fish (freshwater);
- NOEC for crustaceans (freshwater);

- NOEC for algae (freshwater);
- LC_{50} and NOEC for birds;
- NOAEL, LOAEL, CED, NOEC and LOEC carcinogenicity (threshold) data for mammals;
- Carcinogenicity (non-threshold) data for mammals;
- Acute toxicity data for mammals;
- Although some mammalian data is available, any additional data concerning repeated dose data, fertility, maternal-toxicity, development-toxicity and carcinogenicity could improve the risk assessment for human health ;
- Consider running a batch of algae tests using different fresh water and marine algae species to identify whether *Pseudokirchneriella subcapitata* is unusually sensitive
- More accurate data on EU emission rates, concentrations during emissions, and routes of exposure;
- More accurate for concentrations in root, leaf, milk and meat;
- Physical property information on the volatilizing properties of TFA, volatilization from water surfaces is not expected to be an important fate process but it may be higher from dry soil surfaces; and
- Perform a mass balance.

9 Conclusions

HFO-1234yf is the most widely used HFO refrigerant and is being commonly used as a replacement for HFC-134a in mobile air conditioning units. The substance is registered under REACH. HFO-1234ze and HFO-1233zd are also used and have been registered under REACH; both HFO-1234yf and HFO-1233zd have also been registered by the US EPA under the Toxic Substances Control Act (TSCA). A number of other HFO refrigerants were identified as being used or likely to be used, such as HFO-1224yd and HFO-1336mzz, as were a number of HFO/HFC blends. It was established that the impurities present in HFO refrigerants would likely be other HFOs or HFCs, and not other perfluorinated compounds such as PFOS and PFOA, which cannot be generated during the manufacture of HFOs.

Market drivers for the uptake of HFOs globally depend on the phase-down strategies adopted for remaining ODSs and HFCs, together with the future role of 'natural' refrigerants as alternative low-GWP options to HFOs. TEAP has conducted several studies on likely scenarios and these have been leveraged for this work (particularly TEAP XXVII/4 – Annex 4). However, consumption projections only exist up to 2050, so two additional scenarios have been modelled for the period from 2051 – namely a consumption freeze until 2100 and an abrupt phase-out at 2050. The outcome in even the abrupt phase-out case shows legacy emissions beyond 2050 in view of the lifetime of installed equipment and the servicing tail. However, the two scenarios beyond 2050 are believed to display the best and worst cases, providing that the assumptions about demand until 2050 (as shown in the TEAP analysis) are viewed as plausible.

The atmospheric lifetime of HFO-1234yf is estimated to be approximately 6 days (Luecken et al, 2010) compared to HFC-134a with a lifetime of 14 years (Solomon et al, 2016 and references therein). The final atmospheric degradation products of HFOs are dependent on the identity of the HFO, for example, the degradation of HFO-1234yf produces a 100% molar yield of TFA. The degradation products of other HFOs are HF, HCl, formic acid and carbon dioxide.

In the atmosphere, a rapid partitioning of TFA into droplets of clouds, rain and fog occurs (Solomon et al, 2016). Wet precipitation (rain, snow and fog) is assumed to be the major source of TFA in the biosphere, e. g. for Switzerland, it was calculated that wet deposition accounts for 96% of the annual mass flux (Berg et al, 2000). TFA is found in a wide range of water bodies such as rivers, streams, lakes and wetlands where inflow into these water bodies occur from precipitation, glaciers, runoff from land, groundwater (springs) and water-treatment facilities where it forms trifluoroacetate salts (CF_3COO^-) with minerals such as calcium and sodium. About one third of the overall TFA is dislocated by rivers, which results in a considerable amount introduced in terrestrial environments where TFA is susceptible to leaching into the groundwater (Scheurer et al, 2017). There have been few studies on TFA concentrations in groundwater to date but of the few studies that have been conducted, concentrations have been low. This is unexpected as TFA is poorly retained in soil and has large mobility, but may be due to the slow percolation into the groundwater samples that have been tested to date. TFA concentrations in the environment vary with compartment and location with the highest concentrations witnessed in terminal water bodies such as salt lakes, playas and oceans. In freshwaters, TFA is thought to be solely anthropogenic in nature; however, TFA found in oceans is both natural and anthropogenic in source.

Of the tested aquatic organisms, only the alga *Raphidocelis subcapitata* (formally known as *Selenastrum capricornutum* and *Pseudokirchneriella subcapitata*) displayed sensitivity to TFA, although this needs to be confirmed by retesting. However, there is no published data for toxicity to soil macroorganisms except arthropods, terrestrial arthropods or for to birds or soil microorganisms. There is less than satisfactory information on the toxicity of TFA and salts to terrestrial plants, and no studies have been reported for concentrations of TFA in crops for human consumption (Solomon et al. 2016). Furthermore, there is no information on toxicity to organisms found in salt lakes and playas. This is particularly important because salt lakes are the most likely site for accumulation of TFA in the natural environment.

A number of knowledge gaps need to be addressed to conclude that TFA will have negligible effect on the environment. Generally, more research is needed to fully understand the cycle of TFA in the atmosphere and hydrosphere. There is also a lack of information on the amounts of TFA used globally or other potential sources of TFA in the environment i.e. other chemicals with TFA as a degradation product.

The environmental effects of degradation products of HFOs other than TFA are suggested to be minimal. HF is a strong acid but the buffering capacity of surface waters means HF is rapidly neutralised. The concentration of fluoride/chloride produced from the degradation of HFOs (HF/HCl) will have a negligible effect on the total fluoride/chloride flux in the environment. The concentrations of formic acid produced from the degradation of HFOs are expected to be low and will have no impact on organisms; formic acid is a naturally occurring intermediate in the body and ubiquitous in the natural environment (Wallington et al, 2014). CO_2 is a persistent greenhouse gas, however the contribution from this source is negligible compared with the total CO_2 burden.

In regards to human health impacts, ECHA have identified a number of factors needing updating in the REACH dossier for HFO-1234yf. This includes an updated Chemical Safety Report (CSR) with revised DNELs for workers, also a revised exposure assessment for inhalation and risk characterisation for workers or to justify why recommended assessment factors in DNEL derivation were not used, and more information is required on the mutagenicity (ECHA, 2017a). No health hazards have been identified, although information is limited for the health hazards and further work is required (ECHA, 2017e).

However, different algae effect concentrations were identified for particular algae species, this was *Raphidocelis subcapitata* (formally known as *Selenastrum capricornutum* and *Pseudokirchneriella subcapitata*). The effect concentration identified in tests for this algae species were orders of magnitudes lower than that identified for other freshwater and marine algae. In literature it was suggested that this algae may be unusually sensitive and that retesting is needed. Within the REACH registration dossier for some of the TFA *Raphidocelis subcapitata* studies it was also suggested that due to the low number of replicates, EC_{50} for 72h values can only be considered as rough estimates. Some of the other studies submitted as part of the REACH registration dossier also appears to limit tests, some missed important parameters, and in another test the highest concentration used as the greater than EC_{50} only equated to 6% growth inhibition.

A risk assessment was performed for HFO refrigerant use up to the 2100 which was based on the most commonly used HFO substance, HFO-1234yf, and its degradation product, TFA. The risk assessment was performed using EUSES and with a basic PEC:PNEC analysis also performed. The outcome of the risk assessment supported similar conclusions identified in literature, these being that toxicity risk of TFA to organisms and human health appears to be low.

Due to some of the uncertainty and variable results identified for algae, three different sets of EUSES models were run for the scenarios 2025, 2100 phase-out and 2100 plateau, these were with highest algae toxicity data (i.e. most toxic algae data), median average toxicity data and average algae toxicity data. The most toxic algae data result in the highest RCR developed as part of the EUSES risk assessment, the RCRs were significantly higher than median and average algae risk assessments. None of the RCR values for organisms were calculated as being >1, as anticipated this came closest in the 2100 plateau scenario. The 2100 plateau scenario also suggests the highest RCR for TFA entering various environmental compartments. In comparison the 2100 phase-out scenario has the lowest

RCR, however some risk will still remain in the environment due to the long term persistence of TFA and the levels of TFA that have been emitted in previous years. Equally, the lowest MOS for human health was calculated as part of the 2100 plateau scenario, the lowest being for maternal and developmental toxicity. However, the MOS in 2100 plateau was still greater than 100.

Ultimately it appears that TFA is expected to become concentrated in terminal sinks due to TFA being highly persistent. The risk, therefore, increases if emissions of HFO-1234yf to the environment increase. Therefore, phasing out HFOs (and consequently TFA), or emission reduction strategies along with best practise measures that help ensure efficient capturing of HFO/TFA during recycling operations, will help reduce the risk to human and environmental health.

10 Further work

10.1 Identified knowledge gaps

From the results of the literature review and consultation, a number of knowledge gaps requiring further work have been identified and are listed below:

Substance information

- The literature review identified some HFOs that may be used as refrigerants in the future but there is little information available on whether research is ongoing for these refrigerants or whether they will be commercially available in the future;
- HFO blends and their degradation mechanism need to be further researched; and
- The impurities present in HFO refrigerants, such as other HFOs or HFCs, are not identified by manufacturers with only the purity of the named refrigerant being stated.

Chemical processes and degradation products

- In the case of the decomposition of HFO-1234ze, the main decomposition product is listed by a few sources (for example US Environmental Protection Agency, 2016; and Solomon et al, 2016) as TFA; however, the Wallington study (Wallington et al, 2014) lists TFA as an intermediate product; and
- HFO blends and their degradation mechanism need to be further researched.

HFO emissions

- HFO emissions data needs to be readily available and updated on a regular basis;
- When considering the future size of HFO refrigerant market, and consequent emissions, an analysis of the proportion of the market occupied by other low-GWP (‘natural’ refrigerants such as CO_2) needs to be taken into consideration; and
- Additional modelling of HFO emissions could possibly predict dispersion of degradation products and potential hotspots for TFA.

Environmental effects

- There is a lack of case studies investigating the environmental effects of HFO degradation products. For example, periodic temporal monitoring of TFA concentrations in well-known terminal water bodies such as Mono Lake, California, USA and Pyramid Lake, Nevada, USA, and appropriate endorheic basins in Europe would provide an early indication of the rate of TFA accumulation following the large-scale use of HFO-1234yf in MAC;
- More temporal and spatial measurements of TFA in flowing waters and oceans would provide information on trends in concentrations of TFA in these environments;

- There have been few studies on TFA concentrations in groundwater and the potential for bioaccumulation in this compartment. This needs to be addressed due to potential implications for drinking water;

- Further to the previous point, increased sampling of drinking water supplies is needed;

- There is inadequate information on the toxicity of TFA and salts to terrestrial plants. There appears to be no data for toxicity to soil macroorganisms except arthropods, terrestrial arthropods, toxicity to birds or soil microorganisms. The inadequacies for toxicity data for TFA has been highlighted by ECHA and information has been requested to update the registration dossier;

- Although uptake of TFA by plants has been shown, no measurements of the concentrations of TFA in crops for human consumption have been reported;

- There is no information on toxicity to organisms found in salt lakes and playas. This latter uncertainty is particularly important because salt lakes are the most likely site for accumulation of TFA in the natural environment;

- There is limited information on the environmental effects of decomposition products of HFOs other than TFA, where the focus of studies have been;

- More research is needed to fully understand the cycle of TFA in the atmosphere and hydrosphere which has been highlighted as a gap in knowledge at present; and

- There is a lack of information on the amounts of TFA used globally or other potential sources of TFA in the environment.

Human health impacts

- The effect of HFOs on human health need to be studied. There is a lack of publically available information on adverse health effects, the effects of exposure to elevated levels of HFOs and potential side effects of HFOs for workers;

- Thermal decomposition products of HFOs are known, but are not well understood (for example concentrations that could present issues; and

- Information lacking on stoichiometry of intermediate and final products produced from the degradation of HFOs.

Risk assessment

- The risk assessment could be repeated when the REACH registration dossier for TFA has been fully updated by 2021; and

- Other models could be identified to repeat the risk assessment in the future.

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Annex 1 Consultation questions

HFO refrigerants and their degradation products

Based on the outputs of the literature review, relevant questions were devised for consultation, which are as follows:

From our literature review, we have identified HFO-1234yf and HFO-1234ze as being used as refrigerants. Are there emerging HFOs that are likely to be used as refrigerants in the future?

From our literature review, we have identified a number of HFO blends (R-448, R-449, R-450 and R-452). Are there other blends that are being used or likely to be used as refrigerants? What is the composition of these blends?

Do blends of HFOs with HFCs/other substances have technical advantages over purely HFO-based refrigerants? What are these advantages?

In the sub-sectors that you operate in, do you envisage HFO/HFC blend refrigerants will form a greater proportion of the market in the future compared with purely HFO-based refrigerants?

In the sub-sectors that you operate in, what is the projected demand for purely HFO based and HFO/HFC blends refrigerants?

For the HFO substances that you have knowledge of, besides trifluoroacetic acid (TFA), are there other decomposition products that are of interest for each HFO substance? How are these decomposition products dispersed in the atmosphere and in land/water? For the decomposition products (TFA and others) do you have information on their environmental dispersion and toxicological profiles?

For the sub-sectors that you operate in, are you aware of any of the following, and if you are, please can you supply details:

- *Charge levels for HFO refrigerants;*
- *Leakage rates of HFO refrigerants;*
- *Estimates of installed capacities for HFO refrigerants; and*
- *Projected emissions for HFO refrigerants*

What substance impurities are present in your purely HFO-based refrigerants? Do these impurities have any hazards associated with them? Do these impurities contribute to emissions?

What substance impurities are present in your HFO/HFC blend refrigerants? Do these impurities have any hazards associated with them? Do these impurities contribute to emissions?

For individual HFO substances under REACH, the impurities need to be identified. For HFO blends, is there any industry obligation to identify the impurities present or is it sufficient to state the level of purity of the main refrigerant?

Are there any studies that you think would be of interest for this part of the study?

Environmental and human health impacts of HFOs and their degradation products

Based on the outputs of the literature review, relevant questions were devised for consultation to determine the environmental effects of HFOs and degradation products, which are as follows:

From our literature review, we have identified TFA, HF and formic acid as some of the final decomposition products of HFO degradation. Are there other decomposition products of HFOs that are likely to have an environmental impact? Would HFO blends have any additional effects?

What will be the final environmental sinks for TFA, and other identified decomposition products, produced from the degradation of HFOs? Are some ecosystems more likely to be effected than others?

From our literature search, studies suggest that the future production of TFA from the breakdown of HFOs will have a small effect on the total concentration of TFA in the environment. Do you agree with this? Is there uncertainty in this assumption, what's the worst case scenario?

Are the concentrations of TFA resulting from the decomposition of HFOs likely to have an effect on aquatic systems and the wider environment?

Are there any particular organisms or plants vulnerable to TFA accumulation in ecosystems? Are there any particular organisms or plants vulnerable to other degradation products of HFOs such as HF and formic acid?

Is HF produced from the decomposition of HFOs expected to contribute significantly to the total fluoride flux in the environment? Is the HF produced likely to cause acidification of ecosystems?

Are the concentrations of formic acid produced from the decomposition of HFOs likely to have an impact on ecosystems?

Are you aware of any substances/impurities that are produced during the manufacture of HFO refrigerants that may have an environmental impact if released?

During maintenance and at the end-of-life of an article containing HFO refrigerant, are there any environmental impacts associated with the recycling and/or disposal of the article?

For HFO emissions are you aware of any projected emissions for HFOs when used as refrigerants or generally? If you are, please can you supply details.

Are there any studies that you think would be of interest for this part of the study?

Based on the outputs of the literature review, relevant questions were devised for consultation to determine the human health effects of HFOs and degradation products, which are as follows:

What are the associated health effects for workers involved in the production of HFO refrigerants?

What concentrations of HFOs, and other associated hazardous compounds, are workers exposed to? Is there a breakdown per task/activity?

What types of personal protection equipment and local exhaust ventilation is provided for workers?

What are the established guidelines followed by workers for the containment of HFOs after an accidental release or leakage?

From our literature review we have identified the hazardous decomposition products of HFO-1234yf as: carbon monoxide, carbon dioxide, carbonyl halides, hydrogen halides and toxic pyrolysis products that contain fluorine. What are the concentrations of these? Is there additional information on the toxic pyrolysis products that contain fluorine?

For HFO-1234ze, the OEL set by Honeywell is 1000pm 8 hour TWA. How is this measured, and if workers exceed this limit, what is the procedure? Are there OELs in place for other HFO substances and blends?

From our literature review we have identified the hazardous decomposition products of HFO-1234ze as: hydrogen fluoride, fluorocarbons and other fluorine containing compounds. What are the concentrations of these?

What are the associated health effects for workers who are involved in the production of articles containing HFO refrigerants?

Are leakage rates associated with HFO refrigerants used in articles likely to have an environmental impact? Are there any organisms particularly vulnerable if exposed to leaked refrigerants?

Are there any regulations for end-of-life recycling/disposal of the refrigerant? If so, what are the obligations?

During maintenance and at the end-of-life of an article containing HFO refrigerant, are there any human health effects or environmental impacts associated with the recycling and/or disposal of the article?

Are there any studies that you think would be of interest for this part of the study?

Annex 2 Detailed information about methodology

A2.1 Overview of the methodology

The methodology for the study has been divided into the following stages which are discussed in more detail below:

- Task 1: Grey literature search;
- Task 2: Academic literature search;
- Task 3: Screening of the literature using DistillerSR®; and
- Task 4: Consultation

Additionally, the methodology employed for the calculation of the projected emissions and for the risk assessment of HFO refrigerants are also discussed in more detail below:

- Task 5: Project emissions up to 2100; and
- Task 6: Risk assessment up to 2100

For Tasks 5 and 6, the scenarios which have been modelled for post 2050 emissions are:

- Emissions are stabilised after 2050; or
- There is a phase-out of HFO refrigerants after 2050

A2.2 Task 1: Grey literature

Relevant studies for the grey literature were identified from a comprehensive Google search and also a targeted search of relevant agencies, associations and manufacturers of refrigerants; these are detailed below:

- European Chemicals Agency (ECHA) substance information portal;
- Manufacturer websites. This included Arkema, BOC, Chemours, Dupont, Honeywell and MexiChem Flour;
- Met Office;
- Multilateral fund;
- United Nations Environment Programme (UNEP) Technology and Economic Assessment Panel (TEAP) reports;
- United Nations Environment Programme (UNEP) Environmental Effects Assessment Panel (EEAP) reports;
- United Nations International Development Organisation (UNIDO);
- United States Environmental Protection Agency (US EPA); and
- World Meteorological Organization (WMO).

Additional grey literature has also been searched based on consultation responses. The grey literature has been screened for relevance and the relevant data extracted using DistillerSR®, as discussed in Section 2.4. Based on the outcome of one consultation, and after the literature review, the patent database was subsequently searched for impurity information.

A2.3 Task 2: Academic literature

Based on the results obtained from searching the grey literature, the academic literature has been reviewed for relevant studies. Search terms were developed in PubMed. These search terms were broad in scope to ensure a wide range of relevant literature was retrieved. The following search terms were used when searching the literature for HFO substance information, HFO emissions, and chemical processes and degradation products: ((((((((((((((((((((hydrofluoroolefins) OR HFO)) OR ((hydrofluorocarbons refrigerant) OR hfc refrigerant)))))))) OR hfo refrigerant OR hfc refrigerant))) OR ((hydrofluorocarbons emission) OR hfc emission)) AND English[Language]). This search term resulted in 1307 studies being identified. Google Scholar was also reviewed for relevant studies.

For searching literature for environmental and human health impacts, the following search terms were used: ((((((TFA OR trifluoroacetic acid)) AND environmental impact) AND English[Language])) OR environmental impact of hydrofluoroolefins) OR environmental impact of hfo which resulted in 660 studies being identified for the environmental effects and for worker exposure the following search terms were used: (((((((hydrofluoroolefins) OR hfos) AND health)) OR ((hydrofluoroolefin release) OR hfo release)) OR ((hydrofluoroolefin exposure)) which resulted in 214 studies being identified. Google Scholar was also reviewed for relevant studies.

The academic literature has been screened for relevance and the relevant data extracted using DistillerSR®, as discussed in Section 2.4.

A2.4 Task 3: Selection of relevance and data extraction- DistillerSR®

A2.4.1 Screening of the literature

The literature identified during the grey literature and academic literature searches has been scoped for relevance to the study. The selection for relevance stage has been a two stage process based on templates created in DistillerSR®:

1) Screening the title and abstract (Level 1 screening): The titles and abstract were screened for relevance. The question for Level 1 screening was: Is the study reporting on hydrofluoroolefins (HFOs) or HFCs? If the study was relevant or if it was unsure if the study was relevant, these proceeded to Level 2. If the study was on HFCs only, the study was preceded to Level 2 for further checking. Studies which were neither on HFOs or HFCs did not proceed further. For part 2 screening, the question asked was: Is the study reporting on hydrofluoroolefins (HFOs) or TFA? If unsure, take a precautionary approach? If the study was relevant or if it was unsure if the study was relevant, these proceeded to Level 2. Studies that were neither on HFOs or TFA did not proceed further.

2) Screening the full text (Level 2 screening). Six questions were asked at this stage in order to determine the relevance for Part 1. These were: 1) Does the study report on HFOs or HFCs?; 2) Does this study report on any of the following aspects of HFOs: Use of HFOs in refrigerants, chemical processes associated with HFOs, emissions, degradation products (including TFA) and/or sinks and hotspots?; 3) If the study only concerns HFCs, is past/future emissions data present and usable for the study?; 4) Would the study be relevant for Part 2 of this study?; 5) Would the study be relevant for Part 3 (Risk Assessment)?; and 6) Is the study ineligible to be used for the report for any reason?

   For Part 2 of the study, four questions were asked to determine the relevance for Part 2 of the study. These were: 1) Does this study report on any of the following aspects of HFOs:

environmental effects of TFA, decomposition of HFOs and the effect on vulnerable organisms and ecosystems, sinks, hazards to health for elevated levels and leaks, workers health/safety and fire/explosion products?; 2) Would the study be relevant for Part 3 (Risk Assessment)?; 3) Is the study unusable for the report for any reason?; and 4) Why is the study not usable (if answered yes to previous answer)?

A2.4.2 Data extraction

For studies that were relevant after screening, the relevant data was extracted using DistillerSR®. For HFO substance information, HFO emissions, and chemical processes and degradation products, the data extraction has been based on the information required for analysis below:

- Assessing the HFO substances that are used/or likely to be used as refrigerants;
- The chemical processes that are related to the atmospheric fate of individual HFO substances. This includes the atmospheric dispersion, degradation mechanisms and deposition of subsequent degradation products;
- Projected emissions in selected future years with a rough indication of geographical distribution;
- Assessing the degradation products which are most likely to be formed as a result of the use of HFOs;
- How the degradation products disperse in the atmosphere and are deposited to land and water bodies;
- Where the final sinks and hotspots for TFA and other degradations are; and
- Assessing to what extent impurities in commercially available HFOs substances would contribute to pollutant emissions.

For environmental and human health impacts, the data extraction has been based on the information required for analysis below:

- The environmental effects of HFOs and their degradation products including the effects of TFA;
- The environmental effects for vulnerable organisms and ecosystems in locations where pollutants can reach high levels;
- Hazards to health and possible environmental effects related to the accidental release of HFOs or (elevated levels of) regular leaks; and
- Workers health and safety and fire/explosion decomposition products, but not safety aspects.

A2.4.3 Literature review outputs

The figure overleaf summarises the results of the grey and academic literature review for determining the HFO substances that are used or likely to be used as refrigerants, their related emissions, degradation products of HFOs and their atmospheric dispersion. Additional documents were also received from the consultation process after the review of the literature:

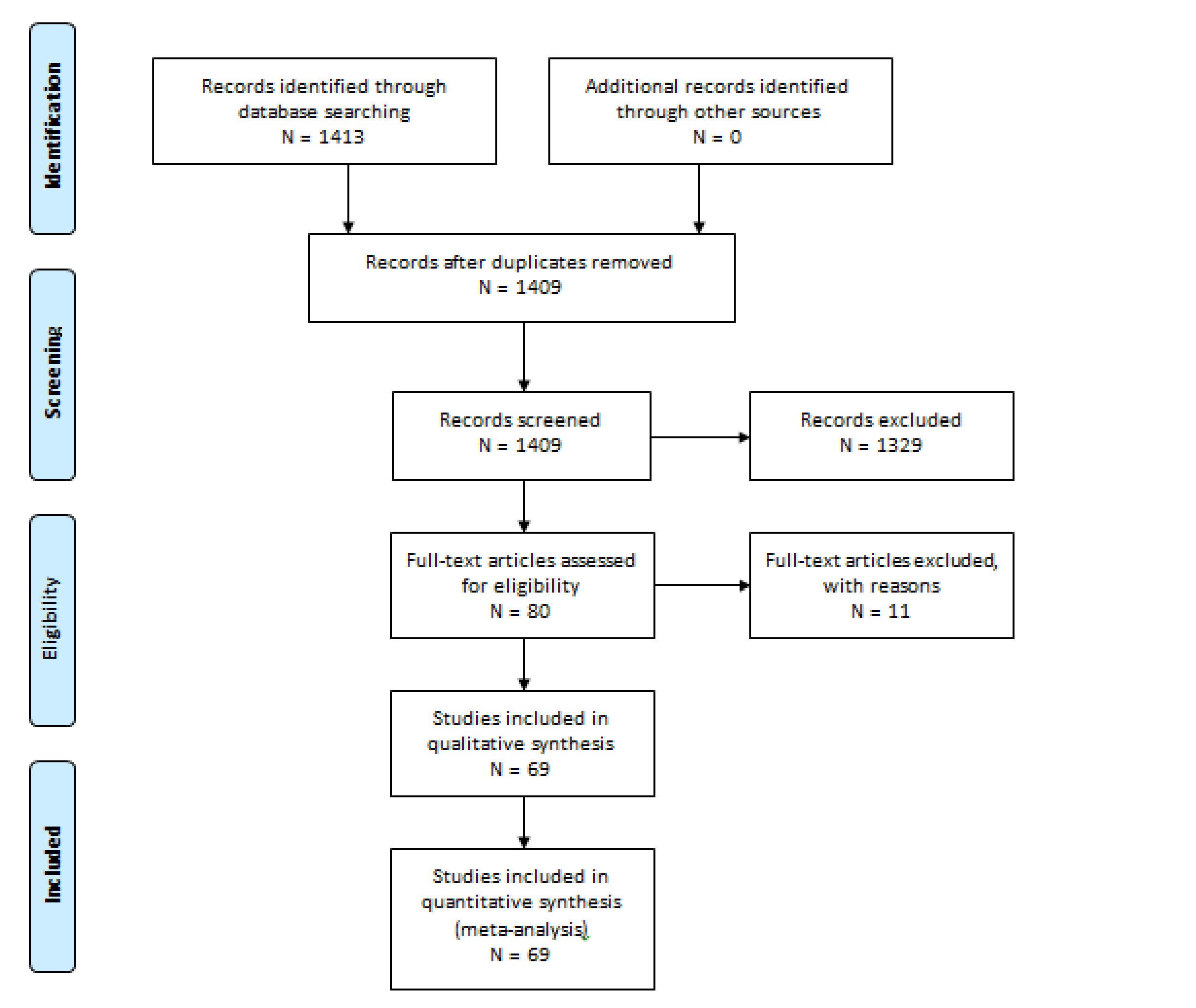


Figure A2-1: PRISMA flowchart for the screening of the identified grey and academic literature for the first part of the study. Source: Moher, D., Liberati, A., Tetzlaff, J., Altman, D.G., The PRISMA Group (2009). Preferred Reporting Items for Systematic Reviews and Meta-Analyses: The PRISMA Statement. PLoS Med 6(6): e1000097. doi:10.1371/journal.pmed1000097

The figure overleaf summarises the results of the grey and academic literature review for assessing the environmental and health effects of HFOs and their degradation products. Additional documents were also received from the consultation process after the review of the literature:

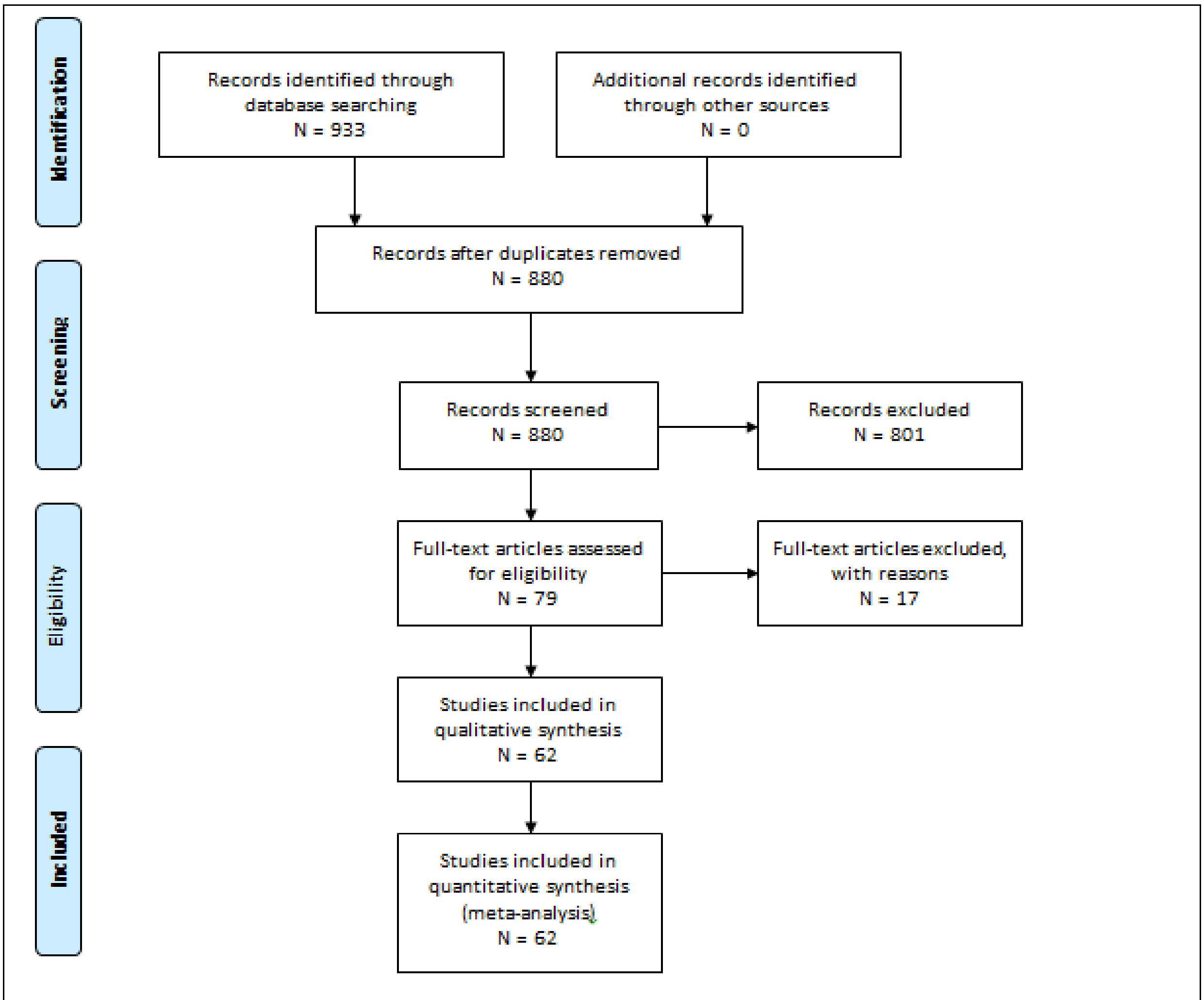


Figure A2-2: PRISMA flowchart for the screening of the identified grey and academic literature for the second part of the study. Source: Moher, D., Liberati, A., Tetzlaff, J., Altman, D.G., The PRISMA Group (2009). Preferred Reporting Items for Systematic Reviews and Meta-Analyses: The PRISMA Statement. PLoS Med 6(6): e1000097. doi:10.1371/journal.pmed1000097

A2.5 Task 4: Consultation

Eight stakeholders were contacted for consultation for the study. These included academic experts, a non-government organisation, a HFO refrigerant manufacturer, a HFO refrigerant reclaimer and a refrigeration industry association. Questions asked during the consultations are listed in Annex 1.

A2.6 Task 5: Assessing HFO projections

A2.6.1 Introduction

The TEAP Task Force Report (XXVII/4) from September 2016 is the most appropriate source for calculating HFO emissions. This was the final TEAP report leading into the Kigali negotiations. The report provides valuable consumption information that we can convert through existing modelling techniques into emission estimates.

The report contains tabulated projected consumption by refrigerant category and RAC (Refrigeration & Air Conditioning) sub-sector in 5 year intervals. From this, it is possible to interpolate for the intervening years and build-up a picture of growth of HFO use, subject to the following:

- Annex 4 only records low-GWP refrigerants as a category, so this would include CO_2, ammonia and hydrocarbons, as well as HFOs;
- Table 2-7 indicates that low-GWP in the terms of the Report means <300 GWP; and
- Tables 2-3 & 2-4 give various pure substances and blends that could qualify.

Annex 4 of the TEAP report also maps at least two Mitigation Scenarios which could be followed in terms of likely low-GWP (Mitigation 5 scenario (MIT-5) and Business As Usual (BAU)). MIT-5 assumes the completion of conversion of key non-Article 5 RAC equipment by 2025 and the commencement of similar conversions in Article 5 countries by the same date.

MIT-5 was viewed as the most representative scenario in respect of the Kigali Amendment that eventually emerged, although even this was marginally too aggressive. However, an over-aggressive schedule would inflate the consumption and emissions of low-GWP alternatives such as HFOs and thereby make the environmental risk assessment appropriately conservative by over-stating consumption and resulting emissions.

Before considering the methodology used for emissions forecasting in detail (see Sections 2.6.2 & 4.2), it is important to also consider the various means by which such emissions models can be verified, at least partially. The most obvious method of verification is by comparison with measured emissions in the atmosphere and the information sources available are highlighted in the following section.

The European Environment Agency reports on the supply, production and emissions of F gases, with the latest publically available report being for the year 2015. The emissions of F-gases accounted for 3% of the overall greenhouse gas emissions in the EU; however owing to confidentiality reasons data is not available for individual substances in the report with only the total for all relevant F-gases reported (European Environment Agency, 2016).

Emissions of HFCs are reported by the European Environment Agency up to 2012 (European Environment Agency, 2015) with emissions of HFCs in 2010 being 81.57 million GWP SAR tonnes, 84.11 million GWP SAR tonnes in 2011 and 85.9 million GWP SAR tonnes in 2012. No information is available for HFO emissions.

HFO emissions are available in the academic literature which is discussed in more detail in the table overleaf.

Table A2-1: HFO emissions data in the literature					
Emission scenario	**HFO substance**	**Measured emissions**	**Projected HFO emissions**	**Methodology used**	**Reference**
For 2020, emissions from HFO-1234yf for vehicles	HFO-1234yf	N/A	11.0 Gg yr^{-1} – 19.2 Gg yr^{-1} in Europe 11.4 Gg yr-[1] to 24.7 Gg yr^{-1} for U.S in 2017	Detailed European emission inventory was developed for 2020 for mobile air conditioning; a complete conversion from HFC-134a to HFO-1234yf was assumed and two emission scenarios developed	Henne, S. et al (2012a): Environmental Impacts of HFO-1234yf and Other HFOs. ASHRAE/NIST Refrigerants Conference
Global HFO emissions	HFO-1234yf, HFO-1234ze(E), HFO-1216, HCFO-1233zd(Z), HCFO-1233zd(E)	N/A	Global assumption of HFO emissions of 100 kt per year	HFO emissions are assumed to be similar to current HFC emissions	Wallington, T.J. et al (2015): Atmospheric chemistry of short-chain haloolefins: photochemical ozone creation potentials (POCPs), global warming potentials (GWPs), and ozone depletion potentials (ODPs). Chemosphere, 129, pp 135-41
Global emissions	HFOs in general	N/A	Global emissions of HCFCs, HFCs, HFEs, and unsaturated HFCs (HFOs) are around 100 kt per year	Emissions have been calculated using the box model. Future emissions are calculated using a fixed annual bank release fraction.	World Meteorological Organization. Scientific Assessment of Ozone Depletion: 2010, Global Ozone Research and Monitoring Project–Report No. 52

Table A2-1: HFO emissions data in the literature					
Emission scenario	**HFO substance**	**Measured emissions**	**Projected HFO emissions**	**Methodology used**	**Reference**
Air emissions measured at two locations in Switzerland (Jungfraujoch and Dubendorf) for 2011-2014	HFO-1234yf HFO-1234ze(E)	Jungfraujoch: For 2011-2013: below limit of detection; 2014: 0.003 mean ppt Dubendorf: For 2013: mean of 0.0032 ppt and for 2014: 0.136 ppt Jungfraujoch: 2011: 0.013 ppt 2012: 0.014 ppt 2013: 0.041 ppt 2014: 0.035 ppt Dubendorf: 2013: 0.704 ppt 2014: 0.928 ppt	From modelling, emissions in Europe in 2020 estimated to be 0.073-15 ppt (mean: 1.5 ppt) for summer and 0.76-29 ppt (mean: 4.1 ppt) for complete conversion in cars to HFO-1234yf	Measurements collected at high altitude (Jungfraujoch) and a laboratory roof-top (Dubendorf) and analysed by Gas Chromatography-Mass Spectrometry (GC-MS)	Vollmer, M. et al (2015): First observations of the fourth generation synthetic halocarbons HFC-1234yf, HFC-1234ze(E), and HCFC-1233zd(E) in the atmosphere. Environ. Sci. Technol., 49, pp 2703-8
Emissions of HFO-1234yf in Japan as refrigerants (discussed in further detail below)	HFO-1234yf	N/A	Estimated as 15,172 tonnes/year in 2050	Future emissions calculated from discharge of HFO-1234yf from air conditioning at each life cycle stage; assumed from 2011 HFO-1234yf is used instead of CFCs/HFCs in all air conditioning equipment.	Kajihara, H. et al (2010): Estimation of environmental concentrations and deposition fluxes of R-1234-YF and its decomposition products emitted from air conditioning equipment to the atmosphere. International Symposium on Next-generation Air Conditioning and

Table A2-1: HFO emissions data in the literature					
Emission scenario	HFO substance	Measured emissions	Projected HFO emissions	Methodology used	Reference
					Refrigeration Technology, 2010

Of course, it should be noted that atmospheric concentration measurements are only useful in validating levels of emission if the modelling of steady state concentrations can be achieved with some confidence. This requires an accurate knowledge of the atmospheric lifetime of each species of HFO refrigerant. The reason why the HFOs have low GWPs is that their average atmospheric lifetime is short. When dealing with short-lifetimes, the actual values can be hard to determine accurately and may vary between geographic locations, depending on the prevailing atmospheric conditions. That said, the tracking of atmospheric concentrations still remains a key tool in 'grounding' emissions forecasts.

In the Kajihara study on refrigerant emissions in Japan, HFO-1234yf refrigerant emissions are discussed in further detail in the table below for the three types of air conditioners used (Kajihara et al, 2010).

Table A2-2: HFO-1234yf refrigerants emissions in Japan in 2050						
Type of A/C		Life-cycle stage of A/C				Total
		Production		Use and Disposal		
		Refrigerants filling at A/C production factory (tonnes/year)	Refrigerants filling at A/C operation location (tonnes/year)	Consumer use (tonnes/year)	Disposal (tonnes/year)	(tonnes/ year)
Home		8	-	1903	4454	6366
Instituti-onal	Stores	5	-	724	1238	1967
	Buildings	2	24	1380	2005	3410
	Facilities	1	2	632	722	1357
Mobile		34	-	1713	325	2072
Total		50	26	6352	8744	15172
Emission coefficients used (-/year)		0.002 for home, institutional and 3 [g/car] for mobile	0.0222 for buildings and 0.0225 for facilities	0.02 for home, 0.03 for stores, 0.035 for buildings, 0.045 for facilities, and 15~100 [g/car/year]	0.73 for home, 0.72 for institutional, and 0.232 for mobile	-
Source: Kajihara, H. et al (2010): Estimation of environmental concentrations and deposition fluxes of R-1234-YF and its decomposition products emitted from air conditioning equipment to the atmosphere. International Symposium on Next-generation Air Conditioning and Refrigeration Technology, 2010						

In correspondence with a manufacturer, HFO-1233zd(E) emissions in terms of organic chlorine have been investigated. In the article from the manufacturer, it is noted that emissions from foams and refrigerants are different, and that if 80% of the HFO-1233zd(E) is used as a blowing foam, then 0.3 ppt of chlorine would be loaded into the atmosphere if consumption is over 200,000 tonnes per year (assuming a background atmospheric loading of 3300 ppt of organic chlorine). No emission estimates are given for their use as refrigerants.

In addition to these published papers, Anthesis-Caleb has worked with UNDP on a series of country level reports which have been based on national HFC Surveys. The countries have been exclusively developing countries supported by funding from the Climate & Clean Air Coalition (CCAC). Since HFC use in these countries is largely restricted to the Refrigeration and Air Conditioning sectors, the modelling work, based on the 2006 IPCC Reporting Guidelines, has provided a good proxy for the conversion of HFC consumption patterns to related emissions.

The overall impact from an environmental perspective can be a little more complex than might at first be perceived, since HFCs (and later HFOs) will ultimately be replacing refrigerants that may have higher GWPs (e.g. HCFC-22). Therefore, the level of greenhouse gas emission from the sector may well decrease over time in GWP-weighted terms. However, to assess the impact of potential breakdown products, it is important to go back to the release by weight of the refrigerants themselves. The following graph for Chile shows the emissions of specific HFCs anticipated to be released in the period to 2030. This analysis also includes the HCFC-22 which will continue to be released from the installed base of equipment, despite its on-going replacement in new equipment.

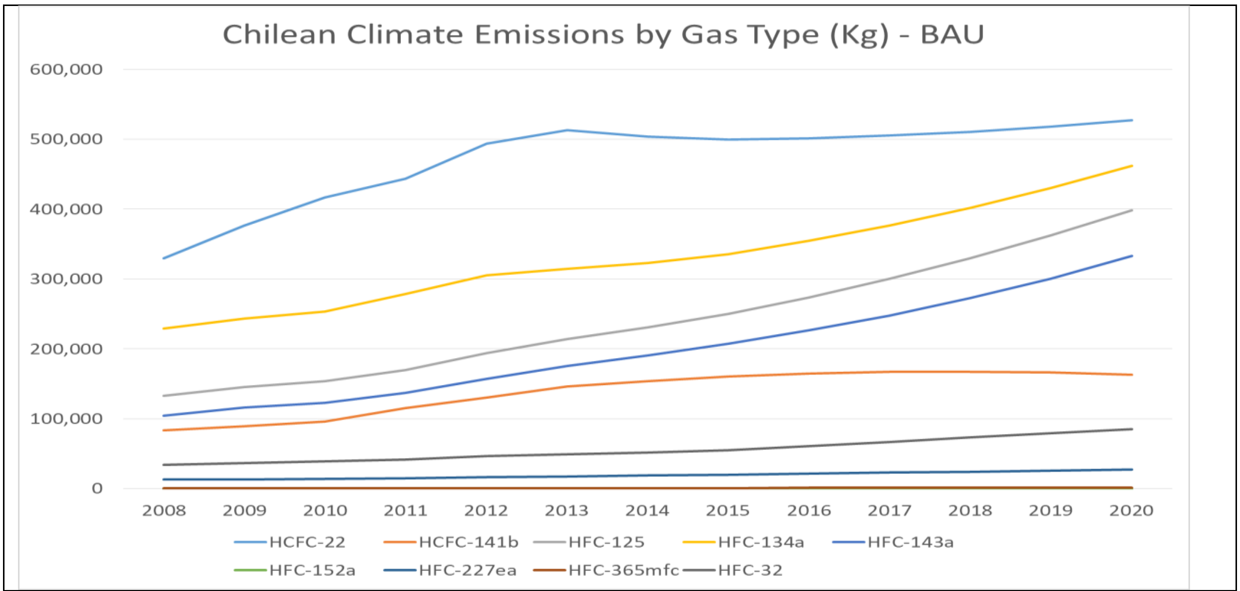


Figure A2-3: Chilean Climate Emissions

For an individual species, the relationship between consumption and emissions is likely to look something like the following:

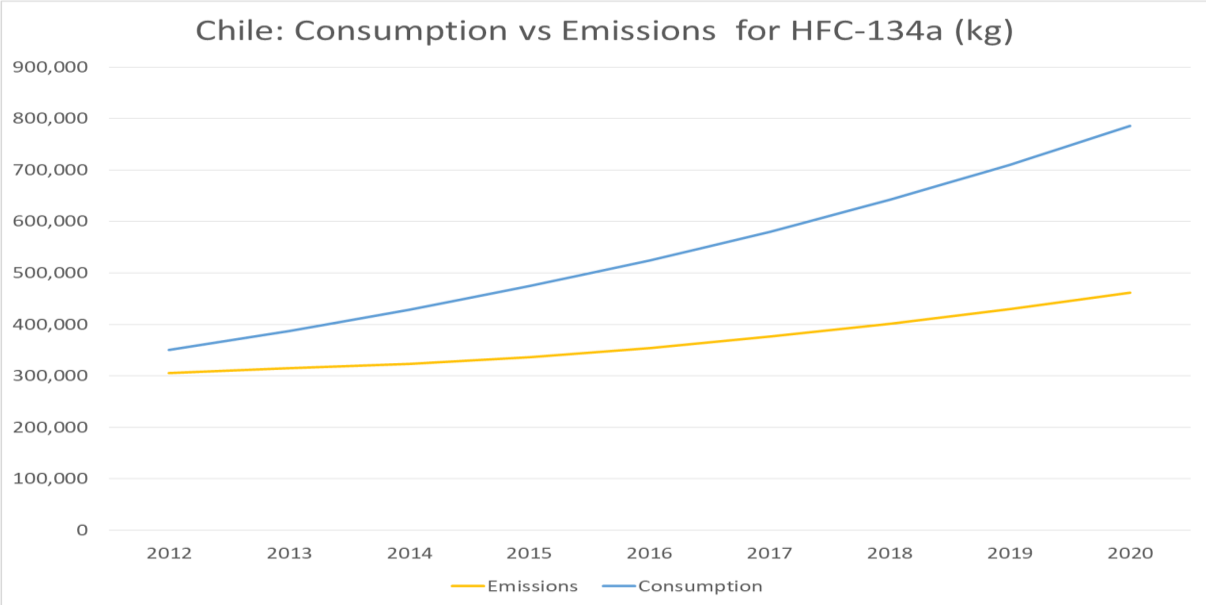


Figure A2-4: Chile: Consumption versus Emissions for HFC-134a

In this instance, the graph illustrates that as the use of HFC-134a moves away from totally emissive applications to contained applications, annual consumption does not have to equal emissions. Indeed, a bank (or reservoir) of HFC builds up in installed equipment and will have its own emission characteristics. As is inferred for HCFC-22 in the earlier graph, annual emissions can outstrip annual consumption when a refrigerant is being phased-out.

A2.6.2 Methodology

The study team used the Tier 2 methodology set out in the 2006 IPCC Reporting guidelines as a basis for calculating emissions of HFOs and used the expertise of Anthesis-Caleb (Coordinating Lead Authors for the ODS Substitutes Chapter of those Guidelines) to develop appropriate high-level models to take advantage of the consumption data contained in Annex 4 of the TEAP XXVII/4 Task Force Report. Since the default emission factors and other assumptions contained in the 2006 Guidelines are now over 10 years old, the following questions were submitted to associations in order to aid the study team in calculating projected emissions:

For the sub-sectors that you operate in, are you aware of any of the following, and if you are, please can you supply details:

- Charge levels for HFO refrigerants;
- Leakage rates of HFO refrigerants;
- Estimates of installed capacities for HFO refrigerants; and
- Projected emissions for HFO refrigerants

In general, awareness of this type of data at the sub-sector level was relatively low amongst respondents, and even where it was available, the regional specificity of the data needed to be recognised when considering whether to apply it to a model which was working on only two global regions (Article 5 and non-Article 5). In the end, expert judgement was used to allocate default emission factors to the various RAC sub-sectors by region. However, the model is sufficiently versatile to be able to adjust those emission factor assessments and thereby allow for further sensitivity analyses to be conducted, should it be required. In keeping with the need to maintain a conservative outlook on atmospheric emissions, relatively high default emission factors were used, seeking to reflect the fact that they cover a range of equipment, some of which might be quite old and leaky. Although the facility exists in the model to reduce the default emission factors year-on-year as the base load of equipment is replaced with newer, and less emissive, equipment, this was not applied in the period up to 2050 (the extent of the data from TEAP). An example of the consumption data used within Annex 4 of the TEAP Report is shown overleaf.

Table A2-3: Consumption data (tonnes) used in Annex 4 of the TEAP report for non-A5 BAU										
Sector	**Substance**	**2010**	**2015**	**2020**	**2025**	**2030**	**2035**	**2040**	**2045**	**2050**
Domestic	HFC-134a	1876	1451	957	954	862	999	1158	1342	1556
	HC-600a	362	415	545	786	1156	1340	1553	1801	2087
Commercial	HFC-134a	2256	2373	2400	2395	2104	2013	2334	2705	3136
	R-404A + R-507	15305	16093	11907	7478	5667	5457	6326	7334	8502
	Low-GWP	0	0	4373	9213	13988	18396	21326	24723	28661
Industrial	HFC-134a	1041	1113	1148	1188	1233	1343	1484	1661	1875
	R-404A + R-507	603	743	491	378	218	193	213	203	178
	R-22	1323	675	455	306	206	139	0	0	0
	Low-GWP	6649	8898	11269	13764	16735	19994	23621	27625	32207
Transport	HFC-134a	222	213	302	371	483	585	679	787	912
	R-404A + R-507	1176	1540	917	833	705	626	588	543	491
	Low-GWP	0	0	557	756	1014	1314	1662	2065	2532
Stationary A/C	HFC-134a	4032	4468	1422	994	226	0	0	0	0
	R-410A	39385	77354	94230	114001	131319	151966	176170	204229	236758
	R-407C	11195	26802	26172	30349	31368	32918	34890	37176	39826
	Low-GWP	0	0	8770	13597	19034	25337	32644	41115	50935
Mobile A/C	HFC-134a	69670	68359	48425	38118	27509	24564	28477	33013	38271
	Low-GWP	0	0	18218	32849	49939	63812	73975	85758	99417
Source: TEAP (2016): TEAP Task Force Report (XXVII/4). Available at: http://conf.montreal-protocol.org/meeting/mop/mop-28/presession/Background%20Documents%20are%20available%20in%20English%20only/TEAP_TFXXVII-4_Report_September2016.pdf										

Further information on emissions is discussed in Section 4 where HFO emissions are projected up to 2100.

A2.7 Task 6: Risk assessment for HFOs

Approach to Assessment

This risk assessment has considered the exposure of the environment to TFA, including the basis for determining the exposure of humans via the environment. Although there is a range of HFO compounds used in the EU, this risk assessment considers the main breakdown product TFA. Although additional exposure assessments could be conducted, encompassing the use of the various other products and their breakdown products, it is anticipated that the assessment of TFA will provide a worst case assessment.

The methodology used for the risk assessment is as follows using EUSES:

- Estimate overall emissions by industry sector (organotin production, glass coating, stabilisers, catalysts and biocides);
- For each sector, estimate emissions by TFA and life-cycle stage (for example, emissions of TFA from different sources); and
- Determine the Predicted Environmental Concentrations (PECs) at a regional level for each of the TFA compounds using the EUSES model

Further information on the inputs for the risk assessment model is discussed in Section 8.

A2.7.1 VEGA

The VEGA platform has been employed to access the QSAR (Quantitative Structure Activity Relationship) models for TFA. The use of QSAR models allows the prediction of the properties of a substance from its structure (VEGA Hub, undated). For TFA, this has been used to examine the mutagenicity, carcinogenicity, development toxicity, fish toxicity, daphnia toxicity, and persistence. Other QSAR models can be used to predict the properties of TFA.

A2.7.2 EUSES

The EUSES (European Union System for the Evaluation of Substances) software has been employed for assessing the environmental and human risks from HFO emissions (EU Science Hub, 2016). The EUSES model generates predicted environmental concentrations (PECs) from estimated releases from use patterns (based on emissions, which is further discussed in section 3) and substance properties (further discussed in Section 4). However, modelling of fluorinated compounds has been challenging. In this assessment a number of challenges were also identified, the calculated values should be used with caution.

Annex 3 TFA VEGA output

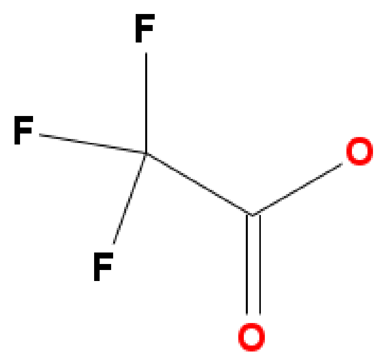
Report

Prediction and Applicability Domain analysis for models:

Mutagenicity (Ames test) CONSENSUS model 1.0.1
Mutagenicity (Ames test) model (CAESAR) 2.1.13
Mutagenicity (Ames test) model (SarPy/IRFMN) 1.0.7
Mutagenicity (Ames test) model (ISS) 1.0.2
Mutagenicity (Ames test) model (KNN/Read-Across) 1.0.0
Carcinogenicity model (CAESAR) 2.1.9
Carcinogenicity model (ISS) 1.0.2
Carcinogenicity model (IRFMN/Antares) 1.0.0
Carcinogenicity model (IRFMN/ISSCAN-CGX) 1.0.0
Developmental Toxicity model (CAESAR) 2.1.7
Developmental/Reproductive Toxicity library (PG) 1.0.0
Estrogen Receptor Relative Binding Affinity model (IRFMN) 1.0.1
Estrogen Receptor-mediated effect (IRFMN/CERAPP) 1.0.0
Skin Sensitization model (CAESAR) 2.1.6
Fish Acute (LC50) Toxicity classification (SarPy/IRFMN) 1.0.2
Fish Acute (LC50) Toxicity model (KNN/Read-Across) 1.0.0
Fish Acute (LC50) Toxicity model (NIC) 1.0.0
Fathead Minnow LC50 96h (EPA) 1.0.7
Daphnia Magna LC50 48h (EPA) 1.0.7
Daphnia Magna LC50 48h (DEMETRA) 1.0.4
Bee acute toxicity model (KNN/IRFMN) 1.0.0
BCF model (CAESAR) 2.1.14
BCF model (Meylan) 1.0.3
BCF model (KNN/Read-Across) 1.1.0
Ready Biodegradability model (IRFMN) 1.0.9
Persistence (sediment) model (IRFMN) 1.0.0
Persistence (soil) model (IRFMN) 1.0.0
Persistence (water) model (IRFMN) 1.0.0
LogP model (Meylan/Kowwin) 1.1.4
LogP model (MLogP) 1.0.0
LogP model (ALogP) 1.0.0

1. Prediction Summary

Prediction for compound Molecule 0



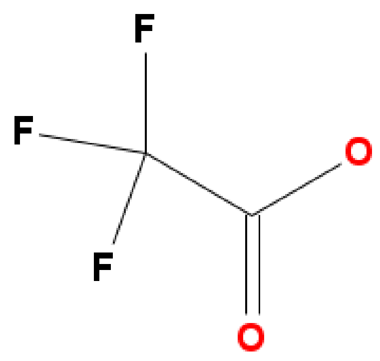
Prediction:

Prediction is NON-Mutagenic with a consensus score of 0.47, based on 4 models.

Compound: Molecule 0
Compound SMILES: O=C(O)C(F)(F)F
Used models: 4
Predicted Consensus Mutagen activity: NON-Mutagenic
Consensus Score: 0.47
Model Caesar assessment: NON-Mutagenic (good reliability)
Model ISS assessment: NON-Mutagenic (low reliability)
Model SarPy assessment: NON-Mutagenic (moderate reliability)
Model KNN assessment: NON-Mutagen (low reliability)
Remarks:
none

1. Prediction Summary

Prediction for compound Molecule 0

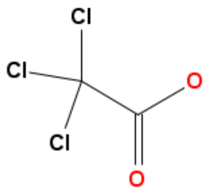


Prediction: Reliability:

Prediction is NON-Mutagenic, the result appears reliable. Anyhow, you should check it through the evaluation of the information given in the following sections. Anyway some issues could be not optimal:
- only moderately similar compounds with known experimental value in the training set have been found

Compound: Molecule 0
Compound SMILES: O=C(O)C(F)(F)F
Experimental value: -
Predicted Mutagen activity: NON-Mutagenic
Structural alerts: -
Reliability: the predicted compound is into the Applicability Domain of the model
Remarks:
none

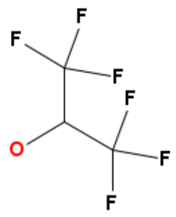
3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



Compound #1

CAS: 76-03-9
Dataset id: 1997 (Test set)
SMILES: O=C(O)C(Cl)(Cl)Cl
Similarity: 0.844

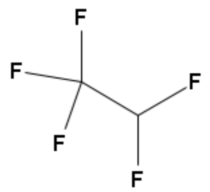
Experimental value: NON-Mutagenic
Predicted value: NON-Mutagenic



Compound #2

CAS: 920-66-1
Dataset id: 3517 (Training set)
SMILES: FC(F)(F)C(O)C(F)(F)F
Similarity: 0.81

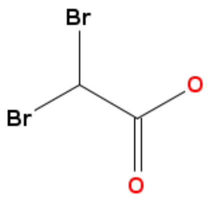
Experimental value: NON-Mutagenic
Predicted value: NON-Mutagenic



Compound #3

CAS: 354-33-6
Dataset id: 3738 (Training set)
SMILES: FC(F)C(F)(F)F
Similarity: 0.794

Experimental value: NON-Mutagenic
Predicted value: NON-Mutagenic

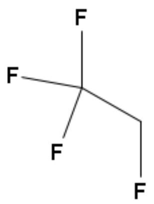


Compound #4

CAS: 631-64-1
Dataset id: 2999 (Test set)
SMILES: O=C(O)C(Br)Br
Similarity: 0.787

Experimental value: Mutagenic
Predicted value: Mutagenic

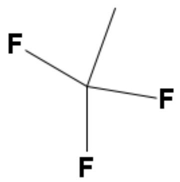
Alerts (not found in the target): SA8 Aliphatic halogens



Compound #5

CAS: 811-97-2
Dataset id: 1244 (Test set)
SMILES: FCC(F)(F)F
Similarity: 0.779

Experimental value: NON-Mutagenic
Predicted value: NON-Mutagenic



Compound #6

CAS: 420-46-2
Dataset id: 2300 (Training set)
SMILES: FC(F)(F)C
Similarity: 0.773

Experimental value: NON-Mutagenic
Predicted value: NON-Mutagenic

3.2 Applicability Domain:
Measured Applicability Domain Scores

Global AD Index
AD index = 0.902
Explanation: the predicted compound is into the Applicability Domain of the model.

Similar molecules with known experimental value
Similarity index = 0.814
Explanation: only moderately similar compounds with known experimental value in the training set have been found.

Accuracy of prediction for similar molecules
Accuracy index = 1
Explanation: accuracy of prediction for similar molecules found in the training set is good.

Concordance for similar molecules
Concordance index = 1
Explanation: similar molecules found in the training set have experimental values that agree with the predicted value.

Model's descriptors range check
Descriptors range check = True
Explanation: descriptors for this compound have values inside the descriptor range of the compounds of the training set.

Atom Centered Fragments similarity check
ACF index = 1
Explanation: all atom centered fragment of the compound have been found in the compounds of the training set.

Symbols explanation:

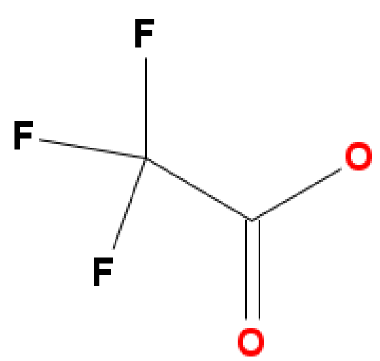
The feature has a good assessment, model is reliable regarding this aspect.

The feature has a non optimal assessment, this aspect should be reviewed by an expert.

The feature has a bad assessment, model is not reliable regarding this aspect.

1. Prediction Summary

Prediction for compound Molecule 0

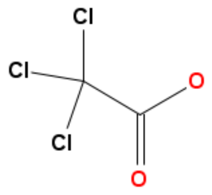


Prediction: Reliability:

Prediction is NON-Mutagenic, but the result shows some critical aspects, which require to be checked:
- accuracy of prediction for similar molecules found in the training set is not optimal
The following relevant fragments have been found: SM150

Compound: Molecule 0
Compound SMILES: O=C(O)C(F)(F)F
Experimental value: -
Predicted Mutagen activity: NON-Mutagenic
No. alerts for mutagenicity: 0
No. alerts for non-mutagenicity: 1
Structural alerts: SM150
Reliability: the predicted compound could be out of the Applicability Domain of the model
Remarks:
none

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values

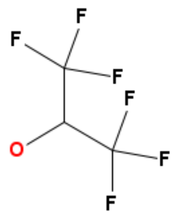


Compound #1

CAS: 76-03-9
Dataset id: 1997 (Test set)
SMILES: O=C(O)C(Cl)(Cl)Cl
Similarity: 0.844

Experimental value: NON-Mutagenic
Predicted value: Mutagenic

Alerts (not found in the target): SM85; SM106

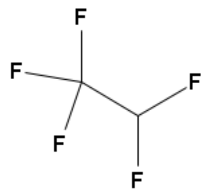


Compound #2

CAS: 920-66-1
Dataset id: 3517 (Training set)
SMILES: FC(F)(F)C(O)C(F)(F)F
Similarity: 0.81

Experimental value: NON-Mutagenic
Predicted value: NON-Mutagenic

Alerts (found also in the target): SM150

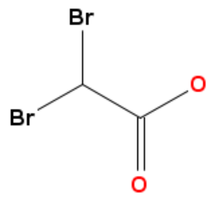


Compound #3

CAS: 354-33-6
Dataset id: 3738 (Training set)
SMILES: FC(F)C(F)(F)F
Similarity: 0.794

Experimental value: NON-Mutagenic
Predicted value: NON-Mutagenic

Alerts (found also in the target): SM150

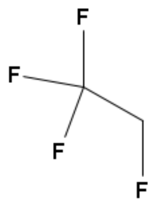


Compound #4

CAS: 631-64-1
Dataset id: 2999 (Test set)
SMILES: O=C(O)C(Br)Br
Similarity: 0.787

Experimental value: Mutagenic
Predicted value: Mutagenic

Alerts (not found in the target): SM93



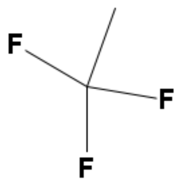
Compound #5

CAS: 811-97-2
Dataset id: 1244 (Test set)
SMILES: FCC(F)(F)F
Similarity: 0.779

Experimental value: NON-Mutagenic
Predicted value: NON-Mutagenic

Alerts (found also in the target): SM150

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



Compound #6

CAS: 420-46-2
Dataset id: 2300 (Training set)
SMILES: FC(F)(F)C
Similarity: 0.773

Experimental value: NON-Mutagenic
Predicted value: NON-Mutagenic

Alerts (found also in the target): SM150

3.2 Applicability Domain:
Measured Applicability Domain Scores

Global AD Index
AD index = 0.811
Explanation: the predicted compound could be out of the Applicability Domain of the model.

Similar molecules with known experimental value
Similarity index = 0.814
Explanation: strongly similar compounds with known experimental value in the training set have been found.

Accuracy of prediction for similar molecules
Accuracy index = 0.652
Explanation: accuracy of prediction for similar molecules found in the training set is not optimal.

Concordance for similar molecules
Concordance index = 1
Explanation: similar molecules found in the training set have experimental values that agree with the predicted value.

Atom Centered Fragments similarity check
ACF index = 1
Explanation: all atom centered fragment of the compound have been found in the compounds of the training set.

Symbols explanation:

The feature has a good assessment, model is reliable regarding this aspect.

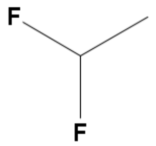
The feature has a non optimal assessment, this aspect should be reviewed by an expert.

The feature has a bad assessment, model is not reliable regarding this aspect.

4.1 Reasoning:
Relevant Chemical Fragments and Moieties

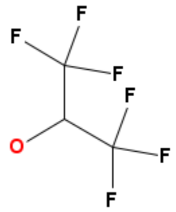
(Molecule 0) Reasoning on fragments/structural alerts:

Fragment found: SM150



Sarpy alert n. 150 for NON-Mutagenicity, defined by the SMARTS: C(F)(F)C

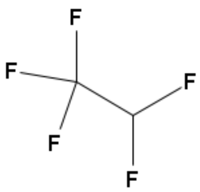
Following, the most similar compounds from the model's dataset having the same fragment.



CAS: 920-66-1
Dataset id: 3517 (Training set)
SMILES: FC(F)(F)C(O)C(F)(F)F
Similarity: 0.81

Experimental value: NON-Mutagenic
Predicted value: NON-Mutagenic

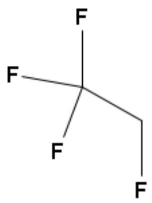
Alerts (found also in the target): SM150



CAS: 354-33-6
Dataset id: 3738 (Training set)
SMILES: FC(F)C(F)(F)F
Similarity: 0.794

Experimental value: NON-Mutagenic
Predicted value: NON-Mutagenic

Alerts (found also in the target): SM150



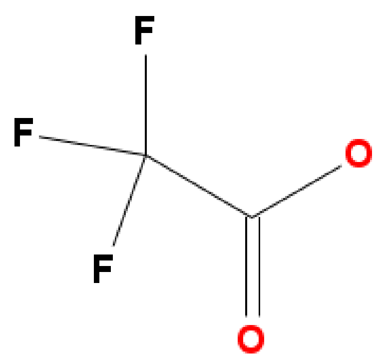
CAS: 811-97-2
Dataset id: 1244 (Test set)
SMILES: FCC(F)(F)F
Similarity: 0.779

Experimental value: NON-Mutagenic
Predicted value: NON-Mutagenic

Alerts (found also in the target): SM150

1. Prediction Summary

Prediction for compound Molecule 0

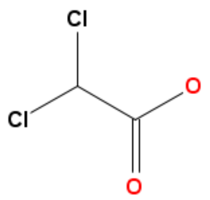


Prediction: Reliability:

Prediction is NON-Mutagenic, but the result may be not reliable. A check of the information given in the following section should be done, paying particular attention to the following issues:
- only moderately similar compounds with known experimental value in the training set have been found
- accuracy of prediction for similar molecules found in the training set is not optimal
- similar molecules found in the training set have experimental values that disagree with the predicted value
- some atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (1 infrequent fragments found)

Compound: Molecule 0
Compound SMILES: O=C(O)C(F)(F)F
Experimental value: -
Predicted Mutagen activity: NON-Mutagenic
Structural alerts: -
Reliability: the predicted compound is outside the Applicability Domain of the model
Remarks:
none

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values

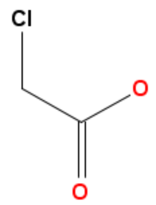


Compound #1

CAS: 79-43-6
Dataset id: 846 (Training set)
SMILES: O=C(O)C(Cl)Cl
Similarity: 0.795

Experimental value: Mutagenic
Predicted value: Mutagenic

Alerts (not found in the target): SA8 Aliphatic halogens

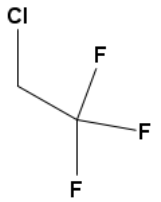


Compound #2

CAS: 79-11-8
Dataset id: 300 (Training set)
SMILES: O=C(O)CCl
Similarity: 0.761

Experimental value: NON-Mutagenic
Predicted value: Mutagenic

Alerts (not found in the target): SA8 Aliphatic halogens

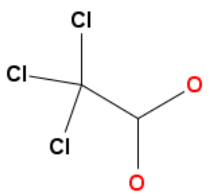


Compound #3

CAS: 75-88-7
Dataset id: 819 (Training set)
SMILES: FC(F)(F)CCl
Similarity: 0.751

Experimental value: NON-Mutagenic
Predicted value: Mutagenic

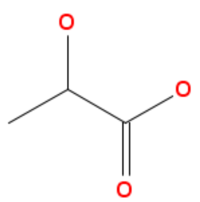
Alerts (not found in the target): SA8 Aliphatic halogens



Compound #4

CAS: 302-17-0
Dataset id: 769 (Training set)
SMILES: OC(O)C(Cl)(Cl)Cl
Similarity: 0.739

Experimental value: Mutagenic
Predicted value: NON-Mutagenic

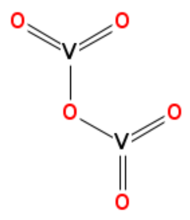


Compound #5

CAS: 814-80-2
Dataset id: 815 (Training set)
SMILES: O=C(O)C(O)C
Similarity: 0.712

Experimental value: NON-Mutagenic
Predicted value: NON-Mutagenic

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



Compound #6

CAS: 1314-62-1
Dataset id: 771 (Training set)
SMILES: O=[V](=O)O[V](=O)=O
Similarity: 0.693

Experimental value: NON-Mutagenic
Predicted value: NON-Mutagenic

3.2 Applicability Domain:
Measured Applicability Domain Scores

Global AD Index
AD index = 0.53
Explanation: the predicted compound is outside the Applicability Domain of the model.

Similar molecules with known experimental value
Similarity index = 0.777
Explanation: only moderately similar compounds with known experimental value in the training set have been found.

Accuracy of prediction for similar molecules
Accuracy index = 0.515
Explanation: accuracy of prediction for similar molecules found in the training set is not optimal.

Concordance for similar molecules
Concordance index = 0.485
Explanation: similar molecules found in the training set have experimental values that disagree with the predicted value.

Atom Centered Fragments similarity check
ACF index = 0.85
Explanation: some atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (1 infrequent fragments found).

Symbols explanation:

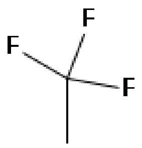
The feature has a good assessment, model is reliable regarding this aspect.

The feature has a non optimal assessment, this aspect should be reviewed by an expert.

The feature has a bad assessment, model is not reliable regarding this aspect.

4.1 Reasoning:
Relevant Chemical Fragments and Moieties

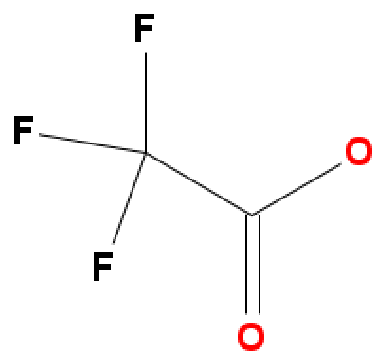
(Molecule 0) Reasoning on rare and missing Atom Centered Fragments.
The following Atom Centered Fragments have been found in the molecule, but they are not found or rarely found in the model's training set:



Fragment defined by the SMILES: FC(F)(F)C
The fragment has less than 3 occurrences in the model's training set

1. Prediction Summary

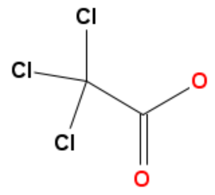
Prediction for compound Molecule 0

	Prediction: Reliability: **Prediction is NON-Mutagen, but the result may be not reliable. A check of the information given in the following section should be done, paying particular attention to the following issues:** **- accuracy of prediction for similar molecules found in the training set is not optimal** **- some similar molecules found in the training set have experimental values that disagree with the predicted value**

Compound: Molecule 0
Compound SMILES: O=C(O)C(F)(F)F
Experimental value: -
Predicted Mutagen activity: NON-Mutagen
Molecules used for prediction: 4
Reliability: the predicted compound is outside the Applicability Domain of the model
Remarks:
none

3.1 Applicability Domain:

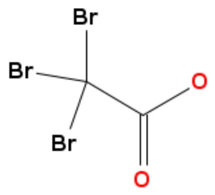
Similar Compounds, with Predicted and Experimental Values



Compound #1

CAS: 76-03-9
Dataset id: 4686 (Training set)
SMILES: O=C(O)C(Cl)(Cl)Cl
Similarity: 0.844

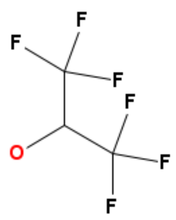
Experimental value: NON-Mutagen
Predicted value: Mutagen



Compound #2

CAS: 75-96-7
Dataset id: 4676 (Training set)
SMILES: O=C(O)C(Br)(Br)Br
Similarity: 0.832

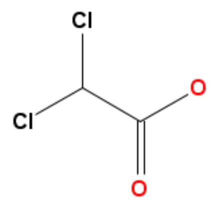
Experimental value: Mutagen
Predicted value: Mutagen



Compound #3

CAS: 920-66-1
Dataset id: 5212 (Training set)
SMILES: FC(F)(F)C(O)C(F)(F)F
Similarity: 0.81

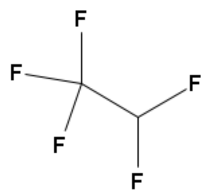
Experimental value: NON-Mutagen
Predicted value: NON-Mutagen



Compound #4

CAS: 79-43-6
Dataset id: 4795 (Training set)
SMILES: O=C(O)C(Cl)Cl
Similarity: 0.795

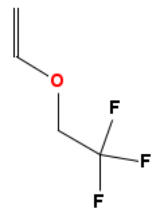
Experimental value: Mutagen
Predicted value: NON-Mutagen



Compound #5

CAS: 354-33-6
Dataset id: 2860 (Training set)
SMILES: FC(F)C(F)(F)F
Similarity: 0.794

Experimental value: NON-Mutagen
Predicted value: NON-Mutagen



Compound #6

CAS: 406-90-6
Dataset id: 3021 (Training set)
SMILES: FC(F)(F)COC=C
Similarity: 0.79

Experimental value: Mutagen
Predicted value: NON-Mutagen

3.2 Applicability Domain:
Measured Applicability Domain Scores

Global AD Index
AD index = 0.641
Explanation: the predicted compound is outside the Applicability Domain of the model.

Similar molecules with known experimental value
Similarity index = 0.818
Explanation: strongly similar compounds with known experimental value in the training set have been found.

Accuracy of prediction for similar molecules
Accuracy index = 0.501
Explanation: accuracy of prediction for similar molecules found in the training set is not optimal.

Concordance for similar molecules
Concordance index = 0.505
Explanation: some similar molecules found in the training set have experimental values that disagree with the predicted value.

Atom Centered Fragments similarity check
ACF index = 1
Explanation: all atom centered fragment of the compound have been found in the compounds of the training set.

Symbols explanation:

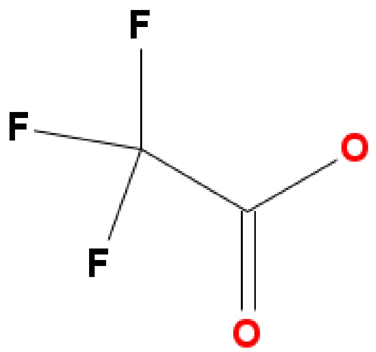
The feature has a good assessment, model is reliable regarding this aspect.

The feature has a non optimal assessment, this aspect should be reviewed by an expert.

The feature has a bad assessment, model is not reliable regarding this aspect.

1. Prediction Summary

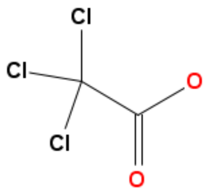
Prediction for compound Molecule 0

	Prediction: Reliability: **Prediction is Carcinogen, but the result may be not reliable. A check of the information given in the following section should be done, paying particular attention to the following issues:** **- accuracy of prediction for similar molecules found in the training set is not adequate** **- similar molecules found in the training set have experimental values that disagree with the predicted value** **- model class assignment is uncertain** **- predicted substance falls into a neuron that is populated by no compounds of the training set**

Compound: Molecule 0
Compound SMILES: O=C(O)C(F)(F)F
Experimental value: -
Predicted Carcinogen activity: Carcinogen
P(Carcinogen): 0.513
P(NON-Carcinogen): 0.487
Reliability: the predicted compound is outside the Applicability Domain of the model
Remarks:
none

3.1 Applicability Domain:

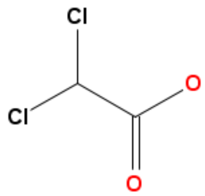
Similar Compounds, with Predicted and Experimental Values



Compound #1

CAS: 76-03-9
Dataset id: 761 (Test set)
SMILES: O=C(O)C(Cl)(Cl)Cl
Similarity: 0.844

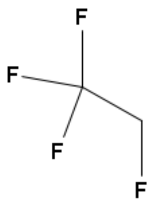
Experimental value: NON-Carcinogen
Predicted value: Carcinogen



Compound #2

CAS: 79-43-6
Dataset id: 219 (Training set)
SMILES: O=C(O)C(Cl)Cl
Similarity: 0.795

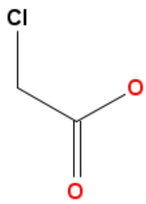
Experimental value: Carcinogen
Predicted value: Carcinogen



Compound #3

CAS: 811-97-2
Dataset id: 729 (Training set)
SMILES: FCC(F)(F)F
Similarity: 0.779

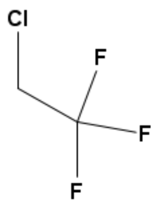
Experimental value: Carcinogen
Predicted value: NON-Carcinogen



Compound #4

CAS: 79-11-8
Dataset id: 487 (Training set)
SMILES: O=C(O)CCl
Similarity: 0.761

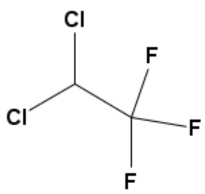
Experimental value: NON-Carcinogen
Predicted value: NON-Carcinogen



Compound #5

CAS: 75-88-7
Dataset id: 148 (Training set)
SMILES: FC(F)(F)CCl
Similarity: 0.751

Experimental value: Carcinogen
Predicted value: Carcinogen



Compound #6

CAS: 306-83-2
Dataset id: 376 (Training set)
SMILES: FC(F)(F)C(Cl)Cl
Similarity: 0.745

Experimental value: Carcinogen
Predicted value: Carcinogen

3.2 Applicability Domain:
Measured Applicability Domain Scores

Global AD Index
AD index = 0
Explanation: the predicted compound is outside the Applicability Domain of the model.

Similar molecules with known experimental value
Similarity index = 0.818
Explanation: strongly similar compounds with known experimental value in the training set have been found.

Accuracy of prediction for similar molecules
Accuracy index = 0.481
Explanation: accuracy of prediction for similar molecules found in the training set is not adequate.

Concordance for similar molecules
Concordance index = 0.481
Explanation: similar molecules found in the training set have experimental values that disagree with the predicted value.

Model's descriptors range check
Descriptors range check = True
Explanation: descriptors for this compound have values inside the descriptor range of the compounds of the training set.

Atom Centered Fragments similarity check
ACF index = 1
Explanation: all atom centered fragment of the compound have been found in the compounds of the training set.

Model class assignment reliability
Pos/Non-Pos difference = 0.026
Explanation: model class assignment is uncertain.

Neural map neurons concordance
Neurons concordance = 0.5
Explanation: predicted substance falls into a neuron that is populated by no compounds of the training set.

Symbols explanation:

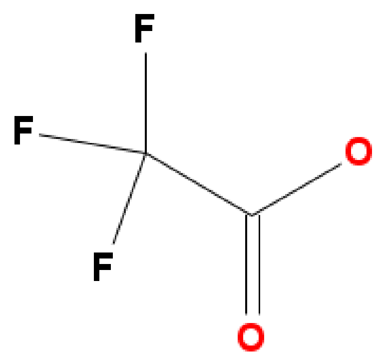
The feature has a good assessment, model is reliable regarding this aspect.

The feature has a non optimal assessment, this aspect should be reviewed by an expert.

The feature has a bad assessment, model is not reliable regarding this aspect.

1. Prediction Summary

Prediction for compound Molecule 0

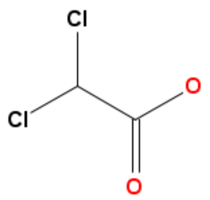
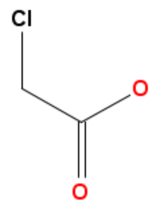
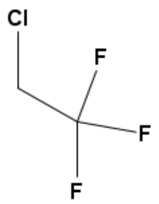
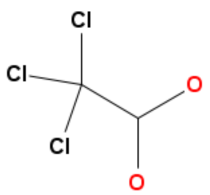
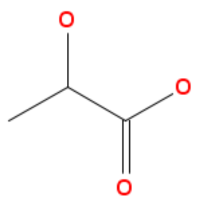


Prediction: Reliability:

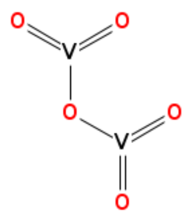
Prediction is NON-Carcinogen, but the result may be not reliable. A check of the information given in the following section should be done, paying particular attention to the following issues:
- only moderately similar compounds with known experimental value in the training set have been found
- accuracy of prediction for similar molecules found in the training set is not optimal
- similar molecules found in the training set have experimental values that disagree with the predicted value

Compound: Molecule 0
Compound SMILES: O=C(O)C(F)(F)F
Experimental value: -
Predicted Carcinogen activity: NON-Carcinogen
Structural alerts: -
Reliability: the predicted compound is outside the Applicability Domain of the model
Remarks:
none

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values

	Compound #1 CAS: 79-43-6 Dataset id: 846 (Training set) SMILES: O=C(O)C(Cl)Cl Similarity: 0.795 Experimental value: Carcinogen Predicted value: Carcinogen Alerts (not found in the target): SA8 Aliphatic halogens
	Compound #2 CAS: 79-11-8 Dataset id: 300 (Training set) SMILES: O=C(O)CCl Similarity: 0.761 Experimental value: NON-Carcinogen Predicted value: Carcinogen Alerts (not found in the target): SA8 Aliphatic halogens
	Compound #3 CAS: 75-88-7 Dataset id: 819 (Training set) SMILES: FC(F)(F)CCl Similarity: 0.751 Experimental value: Carcinogen Predicted value: Carcinogen Alerts (not found in the target): SA8 Aliphatic halogens
	Compound #4 CAS: 302-17-0 Dataset id: 769 (Training set) SMILES: OC(O)C(Cl)(Cl)Cl Similarity: 0.739 Experimental value: Carcinogen Predicted value: Carcinogen Alerts (not found in the target): SA56 Alkyl halides
	Compound #5 CAS: 814-80-2 Dataset id: 815 (Training set) SMILES: O=C(O)C(O)C Similarity: 0.712 Experimental value: NON-Carcinogen Predicted value: NON-Carcinogen

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



Compound #6

CAS: 1314-62-1
Dataset id: 771 (Training set)
SMILES: O=[V](=O)O[V](=O)=O
Similarity: 0.693

Experimental value: Carcinogen
Predicted value: NON-Carcinogen

3.2 Applicability Domain:
Measured Applicability Domain Scores

Global AD Index
AD index = 0.623
Explanation: the predicted compound is outside the Applicability Domain of the model.

Similar molecules with known experimental value
Similarity index = 0.777
Explanation: only moderately similar compounds with known experimental value in the training set have been found.

Accuracy of prediction for similar molecules
Accuracy index = 0.515
Explanation: accuracy of prediction for similar molecules found in the training set is not optimal.

Concordance for similar molecules
Concordance index = 0.485
Explanation: similar molecules found in the training set have experimental values that disagree with the predicted value.

Atom Centered Fragments similarity check
ACF index = 1
Explanation: all atom centered fragment of the compound have been found in the compounds of the training set.

Symbols explanation:

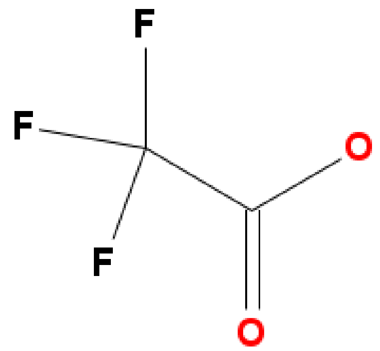
The feature has a good assessment, model is reliable regarding this aspect.

The feature has a non optimal assessment, this aspect should be reviewed by an expert.

The feature has a bad assessment, model is not reliable regarding this aspect.

1. Prediction Summary

Prediction for compound Molecule 0



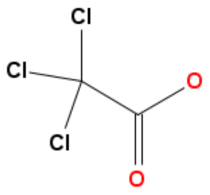
Prediction:

Reliability:

Prediction is Carcinogen, but the result shows some critical aspects, which require to be checked:
- accuracy of prediction for similar molecules found in the training set is not optimal
- some similar molecules found in the training set have experimental values that disagree with the predicted value
The following relevant fragments have been found: Carcinogenity alert no. 125

Compound: Molecule 0
Compound SMILES: O=C(O)C(F)(F)F
Experimental value: -
Predicted Mutagen activity: Carcinogen
No. alerts for carcinogenicity: 1
Structural alerts: Carcinogenity alert no. 125
Reliability: the predicted compound could be out of the Applicability Domain of the model
Remarks:
none

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values

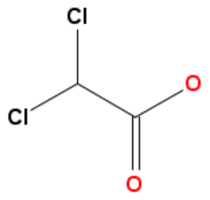


Compound #1

CAS: N.A.
Dataset id: 771 (Training set)
SMILES: O=C(O)C(Cl)(Cl)Cl
Similarity: 0.844

Experimental value: NON-Carcinogen
Predicted value: Carcinogen

Alerts (not found in the target): Carcinogenity alert no. 57

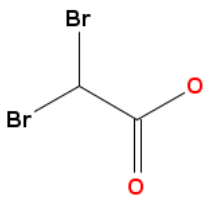


Compound #2

CAS: N.A.
Dataset id: 219 (Training set)
SMILES: O=C(O)C(Cl)Cl
Similarity: 0.795

Experimental value: Carcinogen
Predicted value: Carcinogen

Alerts (not found in the target): Carcinogenity alert no. 57

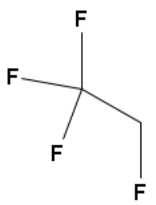


Compound #3

CAS: N.A.
Dataset id: 943 (Training set)
SMILES: O=C(O)C(Br)Br
Similarity: 0.787

Experimental value: Carcinogen
Predicted value: Carcinogen

Alerts (not found in the target): Carcinogenity alert no. 58; Carcinogenity alert no. 59

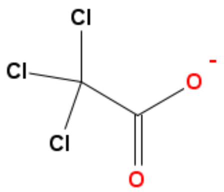


Compound #4

CAS: N.A.
Dataset id: 733 (Training set)
SMILES: FCC(F)(F)F
Similarity: 0.779

Experimental value: Carcinogen
Predicted value: Carcinogen

Alerts (found also in the target): Carcinogenity alert no. 125



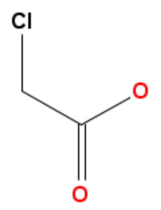
Compound #5

CAS: N.A.
Dataset id: 1058 (Training set)
SMILES: O=C([O-])C(Cl)(Cl)Cl
Similarity: 0.776

Experimental value: NON-Carcinogen
Predicted value: Carcinogen

Alerts (not found in the target): Carcinogenity alert no. 57

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



Compound #6

CAS: N.A.
Dataset id: 486 (Training set)
SMILES: O=C(O)CCl
Similarity: 0.761

Experimental value: NON-Carcinogen
Predicted value: Carcinogen

Alerts (not found in the target): Carcinogenity alert no. 57

3.2 Applicability Domain:

Measured Applicability Domain Scores

Global AD Index
AD index = 0.723
Explanation: the predicted compound could be out of the Applicability Domain of the model.

Similar molecules with known experimental value
Similarity index = 0.806
Explanation: strongly similar compounds with known experimental value in the training set have been found.

Accuracy of prediction for similar molecules
Accuracy index = 0.648
Explanation: accuracy of prediction for similar molecules found in the training set is not optimal.

Concordance for similar molecules
Concordance index = 0.648
Explanation: some similar molecules found in the training set have experimental values that disagree with the predicted value.

Atom Centered Fragments similarity check
ACF index = 1
Explanation: all atom centered fragment of the compound have been found in the compounds of the training set.

Symbols explanation:

The feature has a good assessment, model is reliable regarding this aspect.

The feature has a non optimal assessment, this aspect should be reviewed by an expert.

The feature has a bad assessment, model is not reliable regarding this aspect.

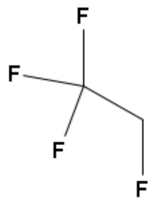
4.1 Reasoning:
Relevant Chemical Fragments and Moieties

(Molecule 0) Reasoning on fragments/structural alerts:

Fragment found: Carcinogenity alert no. 125

Structural alert for carcinogenity defined by the SMARTS: CCF

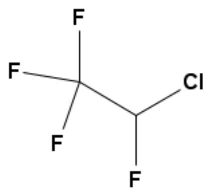
Following, the most similar compounds from the model's dataset having the same fragment.



CAS: N.A.
Dataset id: 733 (Training set)
SMILES: FCC(F)(F)F
Similarity: 0.779

Experimental value: Carcinogen
Predicted value: Carcinogen

Alerts (found also in the target): Carcinogenity alert no. 125

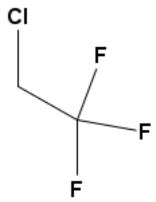


CAS: N.A.
Dataset id: 1398 (Training set)
SMILES: FC(C(F)(F)F)Cl
Similarity: 0.758

Experimental value: NON-Carcinogen
Predicted value: Carcinogen

Alerts (found also in the target): Carcinogenity alert no. 125

Alerts (not found in the target): Carcinogenity alert no. 57



CAS: N.A.
Dataset id: 148 (Training set)
SMILES: FC(F)(F)CCl
Similarity: 0.751

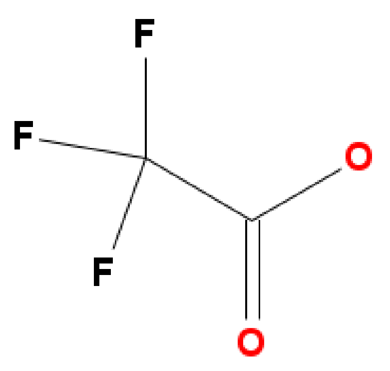
Experimental value: Carcinogen
Predicted value: Carcinogen

Alerts (found also in the target): Carcinogenity alert no. 125

Alerts (not found in the target): Carcinogenity alert no. 57

1. Prediction Summary

Prediction for compound Molecule 0



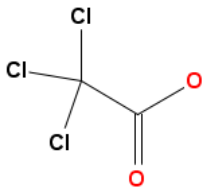
Prediction:

Reliability:

Prediction is Possible NON-Carcinogen, but the result may be not reliable. A check of the information given in the following section should be done, paying particular attention to the following issues:
- only moderately similar compounds with known experimental value in the training set have been found
- accuracy of prediction for similar molecules found in the training set is not adequate
- similar molecules found in the training set have experimental values that disagree with the predicted value

Compound: Molecule 0
Compound SMILES: O=C(O)C(F)(F)F
Experimental value: -
Predicted Mutagen activity: Possible NON-Carcinogen
No. alerts for carcinogenicity: 0
Structural alerts: -
Reliability: the predicted compound is outside the Applicability Domain of the model
Remarks:
none

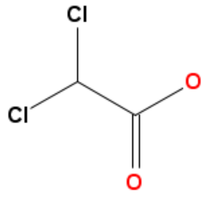
3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



Compound #1

CAS: 76-03-9
Dataset id: 912 (Training set)
SMILES: O=C(O)C(Cl)(Cl)Cl
Similarity: 0.844

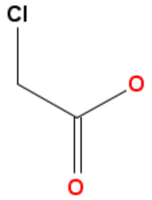
Experimental value: Carcinogen
Predicted value: Possible NON-Carcinogen



Compound #2

CAS: 79-43-6
Dataset id: 627 (Training set)
SMILES: O=C(O)C(Cl)Cl
Similarity: 0.795

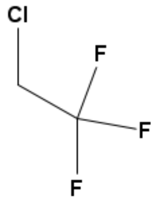
Experimental value: Carcinogen
Predicted value: Possible NON-Carcinogen



Compound #3

CAS: 79-11-8
Dataset id: 242 (Training set)
SMILES: O=C(O)CCl
Similarity: 0.761

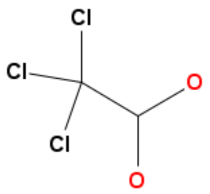
Experimental value: NON-Carcinogen
Predicted value: Possible NON-Carcinogen



Compound #4

CAS: 75-88-7
Dataset id: 617 (Training set)
SMILES: FC(F)(F)CCl
Similarity: 0.751

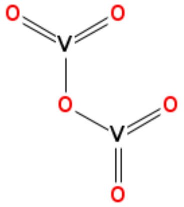
Experimental value: Carcinogen
Predicted value: Possible NON-Carcinogen



Compound #5

CAS: 302-17-0
Dataset id: 598 (Training set)
SMILES: OC(O)C(Cl)(Cl)Cl
Similarity: 0.739

Experimental value: Carcinogen
Predicted value: Possible NON-Carcinogen



Compound #6

CAS: 1314-62-1
Dataset id: 599 (Training set)
SMILES: O=[V](=O)O[V](=O)=O
Similarity: 0.693

Experimental value: Carcinogen
Predicted value: Possible NON-Carcinogen

3.2 Applicability Domain:
Measured Applicability Domain Scores

Global AD Index AD index = 0.498 Explanation: the predicted compound is outside the Applicability Domain of the model.
Similar molecules with known experimental value Similarity index = 0.794 Explanation: only moderately similar compounds with known experimental value in the training set have been found.
Accuracy of prediction for similar molecules Accuracy index = 0.312 Explanation: accuracy of prediction for similar molecules found in the training set is not adequate.
Concordance for similar molecules Concordance index = 0.312 Explanation: similar molecules found in the training set have experimental values that disagree with the predicted value.
Atom Centered Fragments similarity check ACF index = 1 Explanation: all atom centered fragment of the compound have been found in the compounds of the training set.

Symbols explanation:

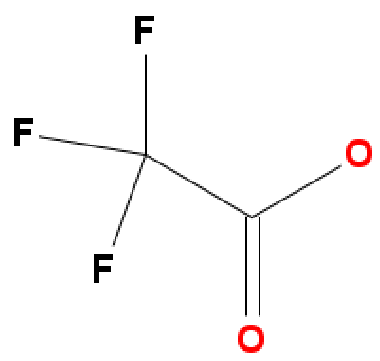
The feature has a good assessment, model is reliable regarding this aspect.

The feature has a non optimal assessment, this aspect should be reviewed by an expert.

The feature has a bad assessment, model is not reliable regarding this aspect.

1. Prediction Summary

Prediction for compound Molecule 0

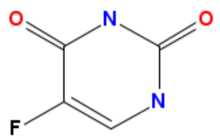


Prediction: Reliability:

Prediction is NON-Toxicant, but the result may be not reliable. A check of the information given in the following section should be done, paying particular attention to the following issues:
- no similar compounds with known experimental value in the training set have been found
- similar molecules found in the training set have experimental values that disagree with the predicted value
- 1 descriptor(s) for this compound have values outside the descriptor range of the compounds of the training set.
- a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (1 unknown fragments found)

Compound: Molecule 0
Compound SMILES: O=C(O)C(F)(F)F
Experimental value: -
Predicted developmental toxicity activity: NON-Toxicant
Reliability: the predicted compound is outside the Applicability Domain of the model
Remarks:
none

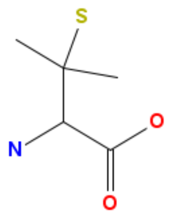
3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



Compound #1

CAS: 51-21-8
Dataset id: 116 (Training set)
SMILES: O=C1NC=C(F)C(=O)N1
Similarity: 0.632

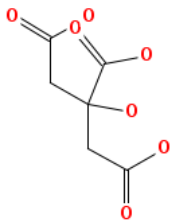
Experimental value: Toxicant
Predicted value: Toxicant



Compound #2

CAS: 52-67-5
Dataset id: 206 (Training set)
SMILES: O=C(O)C(N)C(C)(C)S
Similarity: 0.621

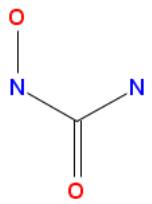
Experimental value: Toxicant
Predicted value: Toxicant



Compound #3

CAS: 866-84-2
Dataset id: 229 (Training set)
SMILES: O=C(O)CC(O)(C(=O)O)CC(=O)O
Similarity: 0.609

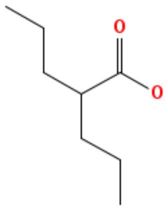
Experimental value: NON-Toxicant
Predicted value: NON-Toxicant



Compound #4

CAS: 127-07-1
Dataset id: 132 (Training set)
SMILES: O=C(N)NO
Similarity: 0.608

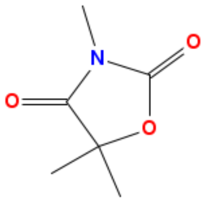
Experimental value: Toxicant
Predicted value: Toxicant



Compound #5

CAS: 99-66-1
Dataset id: 289 (Training set)
SMILES: O=C(O)C(CCC)CCC
Similarity: 0.595

Experimental value: Toxicant
Predicted value: Toxicant



Compound #6

CAS: 127-48-0
Dataset id: 284 (Training set)
SMILES: O=C1OC(C(=O)N1C)(C)C
Similarity: 0.591

Experimental value: Toxicant
Predicted value: Toxicant

3.2 Applicability Domain:
Measured Applicability Domain Scores

Global AD Index
AD index = 0
Explanation: the predicted compound is outside the Applicability Domain of the model.

Similar molecules with known experimental value
Similarity index = 0.626
Explanation: no similar compounds with known experimental value in the training set have been found.

Accuracy of prediction for similar molecules
Accuracy index = 1
Explanation: accuracy of prediction for similar molecules found in the training set is good.

Concordance for similar molecules
Concordance index = 0
Explanation: similar molecules found in the training set have experimental values that disagree with the predicted value.

Model's descriptors range check
Descriptors range check = False
Explanation: 1 descriptor(s) for this compound have values outside the descriptor range of the compounds of the training set..

Atom Centered Fragments similarity check
ACF index = 0.6
Explanation: a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (1 unknown fragments found).

Symbols explanation:

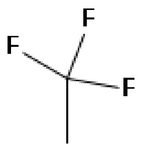
The feature has a good assessment, model is reliable regarding this aspect.

The feature has a non optimal assessment, this aspect should be reviewed by an expert.

The feature has a bad assessment, model is not reliable regarding this aspect.

4.1 Reasoning:
Relevant Chemical Fragments and Moieties

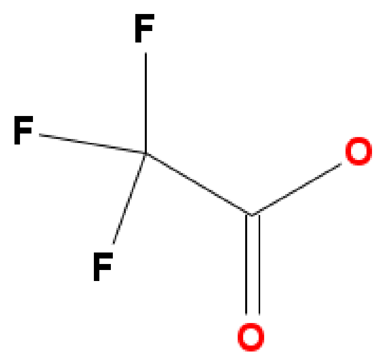
(Molecule 0) Reasoning on rare and missing Atom Centered Fragments.
The following Atom Centered Fragments have been found in the molecule, but they are not found or rarely found in the model's training set:



Fragment defined by the SMILES: FC(F)(F)C
The fragment has never been found in the model's training set

1. Prediction Summary

Prediction for compound Molecule 0



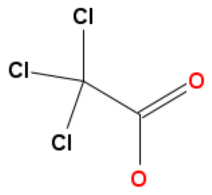
Prediction: Reliability:

Prediction is NON-Toxicant, but the result may be not reliable. A check of the information given in the following section should be done, paying particular attention to the following issues:
- only moderately similar compounds with known experimental value in the training set have been found
- similar molecules found in the training set have experimental values that disagree with the predicted value

Compound: Molecule 0
Compound SMILES: O=C(O)C(F)(F)F
Experimental value: -
Predicted Developmental and Reproductive activity: NON-Toxicant
Matching library description: -
Reliability: the predicted compound is outside the Applicability Domain of the model
Remarks:
none

3.1 Applicability Domain:

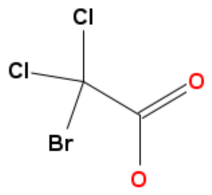
Similar Compounds, with Predicted and Experimental Values



Compound #1

CAS: 76-03-9
Dataset id: 440 (Training set)
SMILES: OC(=O)C(Cl)(Cl)Cl
Similarity: 0.844

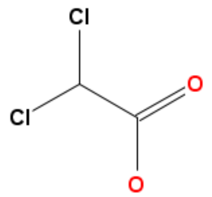
Experimental value: Toxicant
Predicted value: Toxicant



Compound #2

CAS: 71133-14-7
Dataset id: 445 (Training set)
SMILES: OC(=O)C(Cl)(Cl)Br
Similarity: 0.818

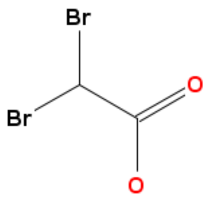
Experimental value: Toxicant
Predicted value: Toxicant



Compound #3

CAS: 79-43-6
Dataset id: 439 (Training set)
SMILES: OC(=O)C(Cl)Cl
Similarity: 0.795

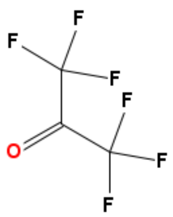
Experimental value: Toxicant
Predicted value: Toxicant



Compound #4

CAS: 631-64-1
Dataset id: 438 (Training set)
SMILES: OC(=O)C(Br)Br
Similarity: 0.787

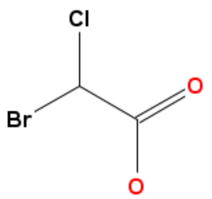
Experimental value: Toxicant
Predicted value: Toxicant



Compound #5

CAS: 684-16-2
Dataset id: 504 (Training set)
SMILES: FC(F)(F)C(=O)C(F)(F)F
Similarity: 0.783

Experimental value: Toxicant
Predicted value: Toxicant



Compound #6

CAS: 5589-96-8
Dataset id: 446 (Training set)
SMILES: OC(=O)C(Cl)Br
Similarity: 0.773

Experimental value: Toxicant
Predicted value: Toxicant

3.2 Applicability Domain:
Measured Applicability Domain Scores

Global AD Index
AD index = 0
Explanation: the predicted compound is outside the Applicability Domain of the model.

Similar molecules with known experimental value
Similarity index = 0.83
Explanation: only moderately similar compounds with known experimental value in the training set have been found.

Accuracy of prediction for similar molecules
Accuracy index = 1
Explanation: accuracy of prediction for similar molecules found in the training set is good.

Concordance for similar molecules
Concordance index = 0
Explanation: similar molecules found in the training set have experimental values that disagree with the predicted value.

Atom Centered Fragments similarity check
ACF index = 1
Explanation: all atom centered fragment of the compound have been found in the compounds of the training set.

Symbols explanation:

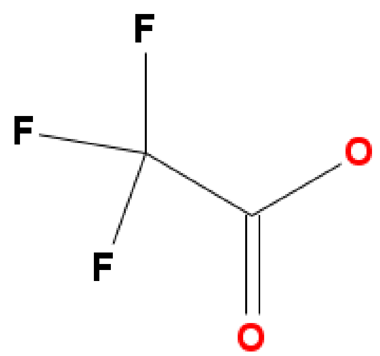
The feature has a good assessment, model is reliable regarding this aspect.

The feature has a non optimal assessment, this aspect should be reviewed by an expert.

The feature has a bad assessment, model is not reliable regarding this aspect.

1. Prediction Summary

Prediction for compound Molecule 0

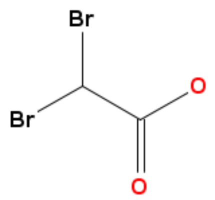


Prediction: Reliability:

Prediction is Inactive, but the result may be not reliable. A check of the information given in the following section should be done, paying particular attention to the following issues:
- only moderately similar compounds with known experimental value in the training set have been found
- 1 descriptor(s) for this compound have values outside the descriptor range of the compounds of the training set.

Compound: Molecule 0
Compound SMILES: O=C(O)C(F)(F)F
Experimental value: -
Predicted activity: Inactive
Classification tree final node: 4
Reliability: the predicted compound is outside the Applicability Domain of the model
Remarks:
none

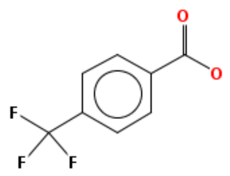
3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



Compound #1

CAS: 631-64-1
Dataset id: 8 (Training set)
SMILES: O=C(O)C(Br)Br
Similarity: 0.787

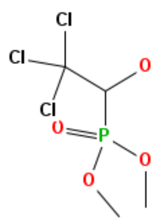
Experimental value: Inactive
Predicted value: Inactive



Compound #2

CAS: 455-24-3
Dataset id: 395 (Training set)
SMILES: O=C(O)c1ccc(cc1)C(F)(F)F
Similarity: 0.679

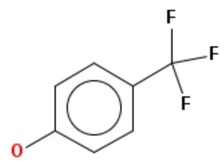
Experimental value: Inactive
Predicted value: Inactive



Compound #3

CAS: 52-68-6
Dataset id: 1 (Training set)
SMILES: O=P(OC)(OC)C(O)C(Cl)(Cl)Cl
Similarity: 0.657

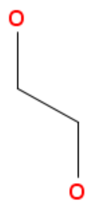
Experimental value: Inactive
Predicted value: Inactive



Compound #4

CAS: 402-45-9
Dataset id: 170 (Training set)
SMILES: FC(F)(F)c1ccc(O)cc1
Similarity: 0.655

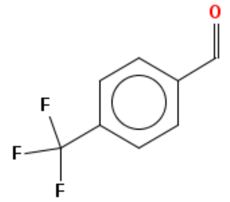
Experimental value: Active
Predicted value: Inactive



Compound #5

CAS: 107-21-1
Dataset id: 22 (Training set)
SMILES: OCCO
Similarity: 0.632

Experimental value: Inactive
Predicted value: Inactive



Compound #6

CAS: 455-19-6
Dataset id: 396 (Training set)
SMILES: O=Cc1ccc(cc1)C(F)(F)F
Similarity: 0.63

Experimental value: Inactive
Predicted value: Inactive

3.2 Applicability Domain:
Measured Applicability Domain Scores

Global AD Index
AD index = 0
Explanation: the predicted compound is outside the Applicability Domain of the model.

Similar molecules with known experimental value
Similarity index = 0.724
Explanation: only moderately similar compounds with known experimental value in the training set have been found.

Accuracy of prediction for similar molecules
Accuracy index = 1
Explanation: accuracy of prediction for similar molecules found in the training set is good.

Concordance for similar molecules
Concordance index = 1
Explanation: similar molecules found in the training set have experimental values that agree with the predicted value.

Model's descriptors range check
Descriptors range check = False
Explanation: 1 descriptor(s) for this compound have values outside the descriptor range of the compounds of the training set..

Atom Centered Fragments similarity check
ACF index = 1
Explanation: all atom centered fragment of the compound have been found in the compounds of the training set.

Symbols explanation:

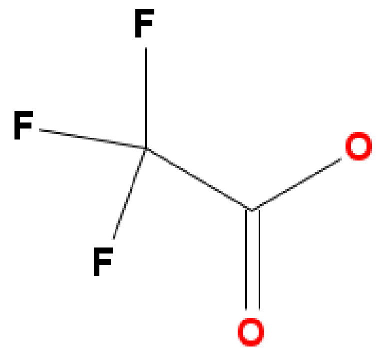
The feature has a good assessment, model is reliable regarding this aspect.

The feature has a non optimal assessment, this aspect should be reviewed by an expert.

The feature has a bad assessment, model is not reliable regarding this aspect.

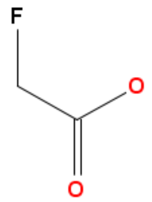
1. Prediction Summary

Prediction for compound Molecule 0

	Prediction: Reliability: **Prediction is Possible NON-active, the result appears reliable. Anyhow, you should check it through the evaluation of the information given in the following sections.** **The following relevant fragments have been found: ER possible non-activity alert no. 9**

Compound: Molecule 0
Compound SMILES: O=C(O)C(F)(F)F
Experimental value: -
Predicted ER-mediated effect: Possible NON-active
No. alerts for activity: 0
No. alerts for possible activity: 0
No. alerts for non-activity: 0
No. alerts for possible non-activity: 1
Structural alerts: ER possible non-activity alert no. 9
Reliability: the predicted compound is into the Applicability Domain of the model
Remarks:
none

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values

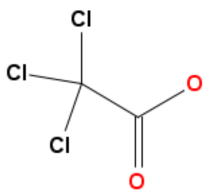


Compound #1

CAS: N.A.
Dataset id: 88 (Training set)
SMILES: O=C(O)CF
Similarity: 0.855

Experimental value: NON-active
Predicted value: Possible NON-active

Alerts (found also in the target): ER possible non-activity alert no. 9



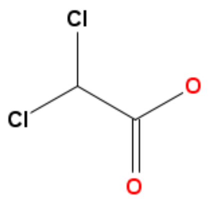
Compound #2

CAS: N.A.
Dataset id: 122 (Training set)
SMILES: O=C(O)C(Cl)(Cl)Cl
Similarity: 0.844

Experimental value: NON-active
Predicted value: NON-active

Alerts (found also in the target): ER possible non-activity alert no. 9

Alerts (not found in the target): ER non-activity alert no. 20



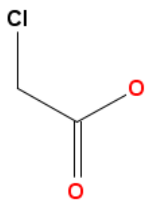
Compound #3

CAS: N.A.
Dataset id: 158 (Training set)
SMILES: O=C(O)C(Cl)Cl
Similarity: 0.795

Experimental value: NON-active
Predicted value: NON-active

Alerts (found also in the target): ER possible non-activity alert no. 9

Alerts (not found in the target): ER non-activity alert no. 20



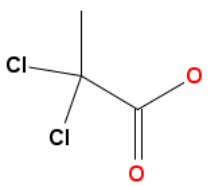
Compound #4

CAS: N.A.
Dataset id: 152 (Training set)
SMILES: O=C(O)CCl
Similarity: 0.761

Experimental value: NON-active
Predicted value: NON-active

Alerts (found also in the target): ER possible non-activity alert no. 9

Alerts (not found in the target): ER non-activity alert no. 20



Compound #5

CAS: N.A.
Dataset id: 121 (Training set)
SMILES: O=C(O)C(C)(Cl)Cl
Similarity: 0.747

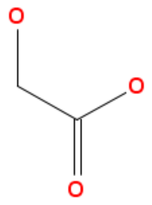
Experimental value: NON-active
Predicted value: NON-active

Alerts (found also in the target): ER possible non-activity alert no. 9

Alerts (not found in the target): ER non-activity alert no. 20

3.1 Applicability Domain:

Similar Compounds, with Predicted and Experimental Values



Compound #6

CAS: N.A.
Dataset id: 153 (Training set)
SMILES: O=C(O)CO
Similarity: 0.73

Experimental value: NON-active
Predicted value: Possible NON-active

Alerts (found also in the target): ER possible non-activity alert no. 9

Alerts (not found in the target): ER possible non-activity alert no. 3

3.2 Applicability Domain:
Measured Applicability Domain Scores

Global AD Index
AD index = 0.91
Explanation: the predicted compound is into the Applicability Domain of the model.

Similar molecules with known experimental value
Similarity index = 0.828
Explanation: strongly similar compounds with known experimental value in the training set have been found.

Accuracy of prediction for similar molecules
Accuracy index = 1
Explanation: accuracy of prediction for similar molecules found in the training set is good.

Concordance for similar molecules
Concordance index = 1
Explanation: similar molecules found in the training set have experimental values that agree with the predicted value.

Atom Centered Fragments similarity check
ACF index = 1
Explanation: all atom centered fragment of the compound have been found in the compounds of the training set.

Symbols explanation:

The feature has a good assessment, model is reliable regarding this aspect.

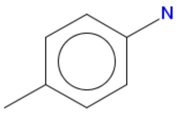
The feature has a non optimal assessment, this aspect should be reviewed by an expert.

The feature has a bad assessment, model is not reliable regarding this aspect.

4.1 Reasoning:
Relevant Chemical Fragments and Moieties

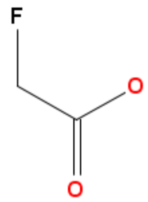
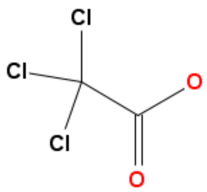
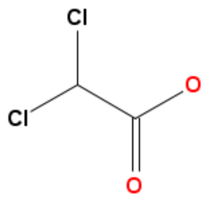
(Molecule 0) Reasoning on fragments/structural alerts:

Fragment found: ER possible non-activity alert no. 9



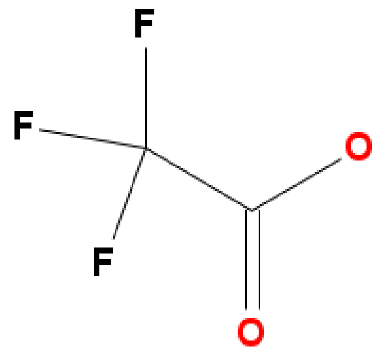
Fragment related to possible non-activity for ER-mediated effect, defined by the SMARTS: C(=O)

Following, the most similar compounds from the model's dataset having the same fragment.

	CAS: N.A. Dataset id: 88 (Training set) SMILES: O=C(O)CF Similarity: 0.855 Experimental value: NON-active Predicted value: Possible NON-active Alerts (found also in the target): ER possible non-activity alert no. 9
	CAS: N.A. Dataset id: 122 (Training set) SMILES: O=C(O)C(Cl)(Cl)Cl Similarity: 0.844 Experimental value: NON-active Predicted value: NON-active Alerts (found also in the target): ER possible non-activity alert no. 9 Alerts (not found in the target): ER non-activity alert no. 20
	CAS: N.A. Dataset id: 158 (Training set) SMILES: O=C(O)C(Cl)Cl Similarity: 0.795 Experimental value: NON-active Predicted value: NON-active Alerts (found also in the target): ER possible non-activity alert no. 9 Alerts (not found in the target): ER non-activity alert no. 20

1. Prediction Summary

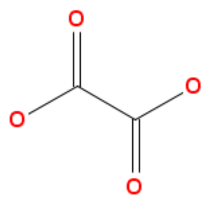
Prediction for compound Molecule 0

<table>
<tr>
<td></td>
<td>Prediction: Reliability:

Prediction is NON-Sensitizer, but the result shows some critical aspects, which require to be checked:
- only moderately similar compounds with known experimental value in the training set have been found
- similar molecules found in the training set have experimental values that disagree with the predicted value
- some atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (2 infrequent fragments found)</td>
</tr>
</table>

Compound: Molecule 0
Compound SMILES: O=C(O)C(F)(F)F
Experimental value: -
Predicted skin sensitization activity: NON-Sensitizer
O(Active): 0.47
O(Inactive): 0.53
Reliability: the predicted compound could be out of the Applicability Domain of the model
Remarks:
none

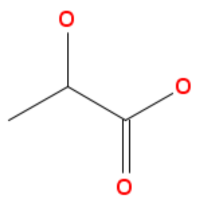
3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



Compound #1

CAS: 144-62-7
Dataset id: 169 (Training set)
SMILES: O=C(O)C(=O)O
Similarity: 0.735

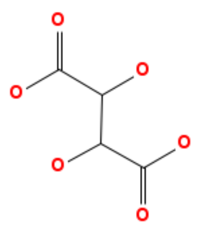
Experimental value: Sensitizer
Predicted value: Sensitizer



Compound #2

CAS: 50-21-5
Dataset id: 127 (Training set)
SMILES: O=C(O)C(O)C
Similarity: 0.712

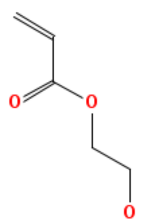
Experimental value: NON-Sensitizer
Predicted value: NON-Sensitizer



Compound #3

CAS: 87-69-4
Dataset id: 196 (Test set)
SMILES: O=C(O)C(O)C(O)C(=O)O
Similarity: 0.654

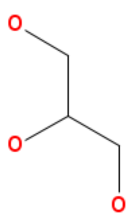
Experimental value: Sensitizer
Predicted value: Sensitizer



Compound #4

CAS: 818-61-1
Dataset id: 110 (Training set)
SMILES: O=C(OCCO)C=C
Similarity: 0.644

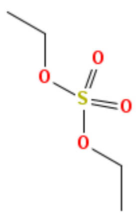
Experimental value: Sensitizer
Predicted value: Sensitizer



Compound #5

CAS: 56-81-5
Dataset id: 102 (Test set)
SMILES: OCC(O)CO
Similarity: 0.629

Experimental value: NON-Sensitizer
Predicted value: NON-Sensitizer



Compound #6

CAS: 64-67-5
Dataset id: 75 (Test set)
SMILES: O=S(=O)(OCC)OCC
Similarity: 0.618

Experimental value: Sensitizer
Predicted value: Sensitizer

3.2 Applicability Domain:
Measured Applicability Domain Scores

Global AD Index
AD index = 0.604
Explanation: the predicted compound could be out of the Applicability Domain of the model.

Similar molecules with known experimental value
Similarity index = 0.723
Explanation: only moderately similar compounds with known experimental value in the training set have been found.

Accuracy of prediction for similar molecules
Accuracy index = 1
Explanation: accuracy of prediction for similar molecules found in the training set is good.

Concordance for similar molecules
Concordance index = 0.488
Explanation: similar molecules found in the training set have experimental values that disagree with the predicted value.

Model's descriptors range check
Descriptors range check = True
Explanation: descriptors for this compound have values inside the descriptor range of the compounds of the training set.

Atom Centered Fragments similarity check
ACF index = 0.85
Explanation: some atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (2 infrequent fragments found).

Symbols explanation:

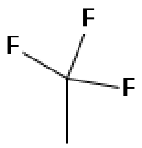
The feature has a good assessment, model is reliable regarding this aspect.

The feature has a non optimal assessment, this aspect should be reviewed by an expert.

The feature has a bad assessment, model is not reliable regarding this aspect.

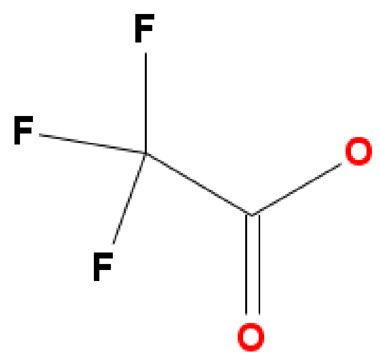
4.1 Reasoning:
Relevant Chemical Fragments and Moieties

(Molecule 0) Reasoning on rare and missing Atom Centered Fragments.
The following Atom Centered Fragments have been found in the molecule, but they are not found or rarely found in the model's training set:

	Fragment defined by the SMILES: FC(F)(F)C The fragment has less than 3 occurrences in the model's training set
	Fragment defined by the SMILES: FC The fragment has less than 3 occurrences in the model's training set

1. Prediction Summary

Prediction for compound Molecule 0

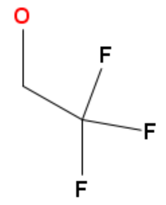


Prediction: Reliability:

Prediction is NON-Toxic (more than 100 mg/l), but the result shows some critical aspects, which require to be checked:
- only moderately similar compounds with known experimental value in the training set have been found
- some atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (1 infrequent fragments found)

Compound: Molecule 0
Compound SMILES: O=C(O)C(F)(F)F
Experimental value: -
Predicted toxicity class: NON-Toxic (more than 100 mg/l)
Structural alerts: -
Reliability: the predicted compound could be out of the Applicability Domain of the model
Remarks:
none

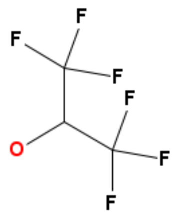
3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



Compound #1

CAS: 75-89-8
Dataset id: 53 (Training set)
SMILES: FC(F)(F)CO
Similarity: 0.872

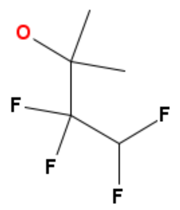
Experimental value: NON-Toxic (more than 100 mg/l)
Predicted value: NON-Toxic (more than 100 mg/l)



Compound #2

CAS: 920-66-1
Dataset id: 413 (Training set)
SMILES: FC(F)(F)C(O)C(F)(F)F
Similarity: 0.81

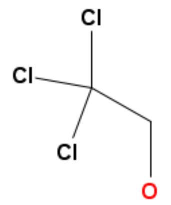
Experimental value: NON-Toxic (more than 100 mg/l)
Predicted value: NON-Toxic (more than 100 mg/l)



Compound #3

CAS: 29553-26-2
Dataset id: 549 (Training set)
SMILES: FC(F)C(F)(F)C(O)(C)C
Similarity: 0.746

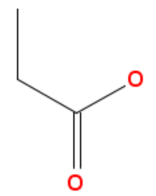
Experimental value: NON-Toxic (more than 100 mg/l)
Predicted value: NON-Toxic (more than 100 mg/l)



Compound #4

CAS: 115-20-8
Dataset id: 243 (Training set)
SMILES: OCC(Cl)(Cl)Cl
Similarity: 0.718

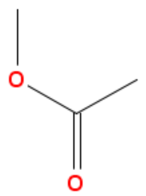
Experimental value: NON-Toxic (more than 100 mg/l)
Predicted value: NON-Toxic (more than 100 mg/l)



Compound #5

CAS: 137-40-6
Dataset id: 286 (Training set)
SMILES: O=C(O)CC
Similarity: 0.702

Experimental value: NON-Toxic (more than 100 mg/l)
Predicted value: NON-Toxic (more than 100 mg/l)



Compound #6

CAS: 79-20-9
Dataset id: 69 (Training set)
SMILES: O=C(OC)C
Similarity: 0.664

Experimental value: NON-Toxic (more than 100 mg/l)
Predicted value: NON-Toxic (more than 100 mg/l)

3.2 Applicability Domain:
Measured Applicability Domain Scores

Global AD Index
AD index = 0.759
Explanation: the predicted compound could be out of the Applicability Domain of the model.

Similar molecules with known experimental value
Similarity index = 0.796
Explanation: only moderately similar compounds with known experimental value in the training set have been found.

Accuracy of prediction for similar molecules
Accuracy index = 1
Explanation: accuracy of prediction for similar molecules found in the training set is good.

Concordance for similar molecules
Concordance index = 1
Explanation: similar molecules found in the training set have experimental values that agree with the predicted value.

Atom Centered Fragments similarity check
ACF index = 0.85
Explanation: some atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (1 infrequent fragments found).

Symbols explanation:

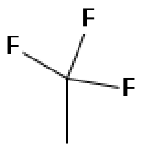
The feature has a good assessment, model is reliable regarding this aspect.

The feature has a non optimal assessment, this aspect should be reviewed by an expert.

The feature has a bad assessment, model is not reliable regarding this aspect.

4.1 Reasoning:
Relevant Chemical Fragments and Moieties

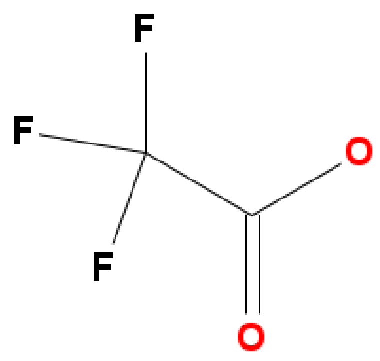
(Molecule 0) Reasoning on rare and missing Atom Centered Fragments.
The following Atom Centered Fragments have been found in the molecule, but they are not found or rarely found in the model's training set:



Fragment defined by the SMILES: FC(F)(F)C
The fragment has less than 3 occurrences in the model's training set

1. Prediction Summary

Prediction for compound Molecule 0

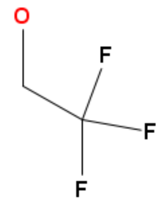


Prediction: Reliability:

Prediction is 177.19 mg/L, but the result shows some critical aspects, which require to be checked:
- the maximum error in prediction of similar molecules found in the training set has a moderate value, considering the experimental variability

Compound: Molecule 0
Compound SMILES: O=C(O)C(F)(F)F
Experimental value [-log(mg/L)]: -
Predicted toxicity [-log(mg/L)]: -2.25
Predicted toxicity [mg/L]: 177.19
Molecules used for prediction: 4
Experimental value [mg/l]: -
Reliability: the predicted compound could be out of the Applicability Domain of the model
Remarks:
none

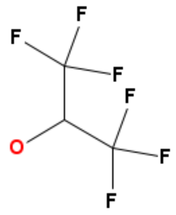
3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



Compound #1

CAS: 000075-89-8
Dataset id: 84 (Training set)
SMILES: FC(F)(F)CO
Similarity: 0.872

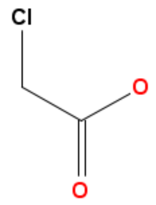
Experimental value [-log(mg/L)]: -2.077
Predicted value [-log(mg/L)]: -1.862



Compound #2

CAS: 000920-66-1
Dataset id: 86 (Training set)
SMILES: FC(F)(F)C(O)C(F)(F)F
Similarity: 0.81

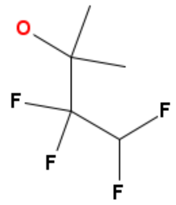
Experimental value [-log(mg/L)]: -2.386
Predicted value [-log(mg/L)]: -1.88



Compound #3

CAS: 000079-11-8
Dataset id: 241 (Training set)
SMILES: O=C(O)CCl
Similarity: 0.761

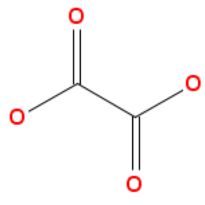
Experimental value [-log(mg/L)]: -1.856
Predicted value [-log(mg/L)]: -2.173



Compound #4

CAS: 029553-26-2
Dataset id: 85 (Training set)
SMILES: FC(F)C(F)(F)C(O)(C)C
Similarity: 0.746

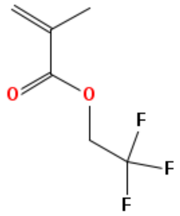
Experimental value [-log(mg/L)]: -2.763
Predicted value [-log(mg/L)]: -1.902



Compound #5

CAS: 000144-62-7
Dataset id: 236 (Training set)
SMILES: O=C(O)C(=O)O
Similarity: 0.735

Experimental value [-log(mg/L)]: -1.43
Predicted value [-log(mg/L)]: -1.726



Compound #6

CAS: 000352-87-4
Dataset id: 218 (Training set)
SMILES: O=C(OCC(F)(F)F)C(=C)C
Similarity: 0.732

Experimental value [-log(mg/L)]: -0.918
Predicted value [-log(mg/L)]: -1.081

3.2 Applicability Domain:

Measured Applicability Domain Scores

Global AD Index AD index = 0.85 Explanation: the predicted compound could be out of the Applicability Domain of the model.

Similar molecules with known experimental value Similarity index = 0.785 Explanation: strongly similar compounds with known experimental value in the training set have been found.
Accuracy of prediction for similar molecules Accuracy index = 0.474 Explanation: accuracy of prediction for similar molecules found in the training set is good.
Concordance for similar molecules Concordance index = 0.304 Explanation: similar molecules found in the training set have experimental values that agree with the predicted value.
Maximum error of prediction among similar molecules Max error index = 0.861 Explanation: the maximum error in prediction of similar molecules found in the training set has a moderate value, considering the experimental variability.
Atom Centered Fragments similarity check ACF index = 1 Explanation: all atom centered fragment of the compound have been found in the compounds of the training set.

Symbols explanation:

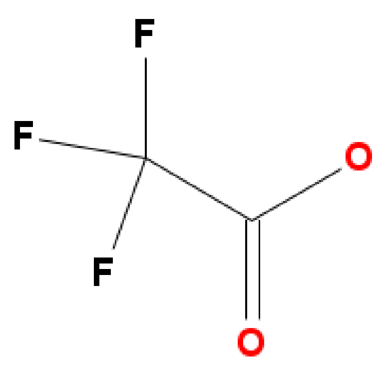
The feature has a good assessment, model is reliable regarding this aspect.

The feature has a non optimal assessment, this aspect should be reviewed by an expert.

The feature has a bad assessment, model is not reliable regarding this aspect.

1. Prediction Summary

Prediction for compound Molecule 0

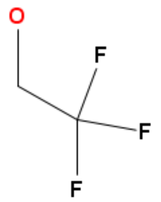


Prediction: Reliability:

Prediction is 244.67 mg/L, but the result shows some critical aspects, which require to be checked:
- only moderately similar compounds with known experimental value in the training set have been found

Compound: Molecule 0
Compound SMILES: O=C(O)C(F)(F)F
Experimental value [log(1/(mmol/L))]: -
Predicted fish toxicity [log(1/(mmol/L))]: -0.33
Predicted fish toxicity [mg/l]: 244.67
Molecular Weight: 113.86
Experimental value [mg/l]: -
Reliability: the predicted compound could be out of the Applicability Domain of the model
Remarks:
none

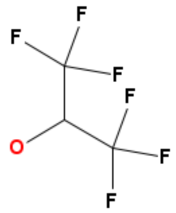
3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



Compound #1

CAS: 000075-89-8
Dataset id: 84 (Training set)
SMILES: FC(F)(F)CO
Similarity: 0.872

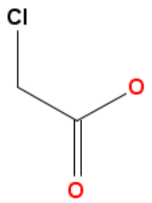
Experimental value [log(1/(mmol/L))]: -0.078
Predicted value [log(1/(mmol/L))]: -0.332



Compound #2

CAS: 000920-66-1
Dataset id: 86 (Test set)
SMILES: FC(F)(F)C(O)C(F)(F)F
Similarity: 0.81

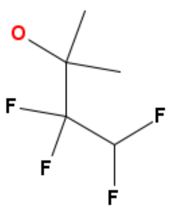
Experimental value [log(1/(mmol/L))]: -0.161
Predicted value [log(1/(mmol/L))]: -0.332



Compound #3

CAS: 000079-11-8
Dataset id: 241 (Test set)
SMILES: O=C(O)CCl
Similarity: 0.761

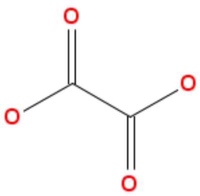
Experimental value [log(1/(mmol/L))]: 0.118
Predicted value [log(1/(mmol/L))]: -0.007



Compound #4

CAS: 029553-26-2
Dataset id: 85 (Training set)
SMILES: FC(F)C(F)(F)C(O)(C)C
Similarity: 0.746

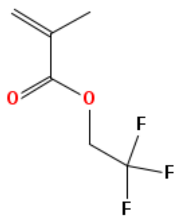
Experimental value [log(1/(mmol/L))]: -0.56
Predicted value [log(1/(mmol/L))]: -0.332



Compound #5

CAS: 000144-62-7
Dataset id: 236 (Test set)
SMILES: O=C(O)C(=O)O
Similarity: 0.735

Experimental value [log(1/(mmol/L))]: 0.523
Predicted value [log(1/(mmol/L))]: -0.008



Compound #6

CAS: 000352-87-4
Dataset id: 218 (Training set)
SMILES: O=C(OCC(F)(F)F)C(=C)C
Similarity: 0.732

Experimental value [log(1/(mmol/L))]: 1.307
Predicted value [log(1/(mmol/L))]: 1.206

3.2 Applicability Domain:
Measured Applicability Domain Scores

Global AD Index
AD index = 0.85
Explanation: the predicted compound could be out of the Applicability Domain of the model.

Similar molecules with known experimental value
Similarity index = 0.838
Explanation: only moderately similar compounds with known experimental value in the training set have been found.

Accuracy of prediction for similar molecules
Accuracy index = 0.213
Explanation: accuracy of prediction for similar molecules found in the training set is good.

Concordance for similar molecules
Concordance index = 0.213
Explanation: similar molecules found in the training set have experimental values that agree with the predicted value.

Maximum error of prediction among similar molecules
Max error index = 0.254
Explanation: the maximum error in prediction of similar molecules found in the training set has a low value, considering the experimental variability.

Model's descriptors range check
Descriptors range check = True
Explanation: descriptors for this compound have values inside the descriptor range of the compounds of the training set.

Atom Centered Fragments similarity check
ACF index = 1
Explanation: all atom centered fragment of the compound have been found in the compounds of the training set.

Symbols explanation:

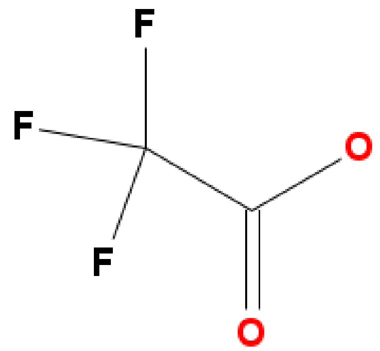
The feature has a good assessment, model is reliable regarding this aspect.

The feature has a non optimal assessment, this aspect should be reviewed by an expert.

The feature has a bad assessment, model is not reliable regarding this aspect.

1. Prediction Summary

Prediction for compound Molecule 0



Prediction:

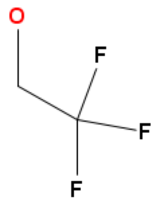
Reliability:

Prediction is 290.52 mg/L, but the result shows some critical aspects, which require to be checked:
- accuracy of prediction for similar molecules found in the training set is not optimal
- the maximum error in prediction of similar molecules found in the training set has a moderate value, considering the experimental variability

Compound: Molecule 0
Compound SMILES: O=C(O)C(F)(F)F
Experimental value [-log(mol/l)]: -
Predicted toxicity [-log(mol/l)]: 2.59
Predicted toxicity [mg/l]: 290.52
Molecular Weight: 113.86
Experimental value [mg/l]: -
Reliability: the predicted compound could be out of the Applicability Domain of the model
Remarks:
none

3.1 Applicability Domain:

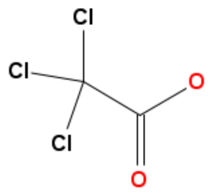
Similar Compounds, with Predicted and Experimental Values



Compound #1

CAS: 75-89-8
Dataset id: 55 (Training set)
SMILES: FC(F)(F)CO
Similarity: 0.872

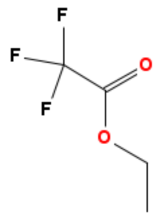
Experimental value [-log(mol/l)]: 2.93
Predicted value [-log(mol/l)]: 2.108



Compound #2

CAS: 76-03-9
Dataset id: 57 (Training set)
SMILES: O=C(O)C(Cl)(Cl)Cl
Similarity: 0.844

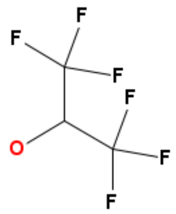
Experimental value [-log(mol/l)]: 1.91
Predicted value [-log(mol/l)]: 3.001



Compound #3

CAS: 383-63-1
Dataset id: 353 (Training set)
SMILES: O=C(OCC)C(F)(F)F
Similarity: 0.84

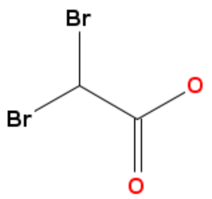
Experimental value [-log(mol/l)]: 1.15
Predicted value [-log(mol/l)]: 2.958



Compound #4

CAS: 920-66-1
Dataset id: 456 (Training set)
SMILES: FC(F)(F)C(O)C(F)(F)F
Similarity: 0.81

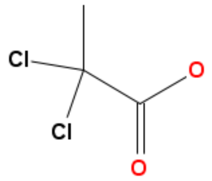
Experimental value [-log(mol/l)]: 2.84
Predicted value [-log(mol/l)]: 3.136



Compound #5

CAS: 631-64-1
Dataset id: 424 (Training set)
SMILES: O=C(O)C(Br)Br
Similarity: 0.787

Experimental value [-log(mol/l)]: 3.5
Predicted value [-log(mol/l)]: 3.97



Compound #6

CAS: 75-99-0
Dataset id: 662 (Test set)
SMILES: O=C(O)C(C)(Cl)Cl
Similarity: 0.747

Experimental value [-log(mol/l)]: 2.69
Predicted value [-log(mol/l)]: 2.806

3.2 Applicability Domain:
Measured Applicability Domain Scores

Global AD Index
AD index = 0.85
Explanation: the predicted compound could be out of the Applicability Domain of the model.

Similar molecules with known experimental value
Similarity index = 0.857
Explanation: strongly similar compounds with known experimental value in the training set have been found.

Accuracy of prediction for similar molecules
Accuracy index = 0.956
Explanation: accuracy of prediction for similar molecules found in the training set is not optimal.

Concordance for similar molecules
Concordance index = 0.51
Explanation: similar molecules found in the training set have experimental values that agree with the predicted value.

Maximum error of prediction among similar molecules
Max error index = 1.091
Explanation: the maximum error in prediction of similar molecules found in the training set has a moderate value, considering the experimental variability.

Model's descriptors range check
Descriptors range check = True
Explanation: descriptors for this compound have values inside the descriptor range of the compounds of the training set.

Atom Centered Fragments similarity check
ACF index = 1
Explanation: all atom centered fragment of the compound have been found in the compounds of the training set.

Symbols explanation:

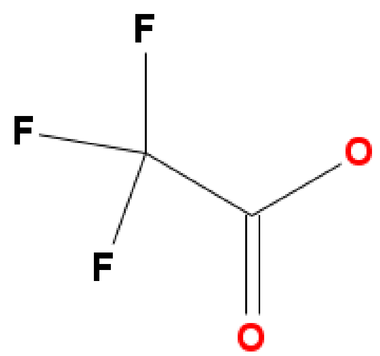
The feature has a good assessment, model is reliable regarding this aspect.

The feature has a non optimal assessment, this aspect should be reviewed by an expert.

The feature has a bad assessment, model is not reliable regarding this aspect.

1. Prediction Summary

Prediction for compound Molecule 0

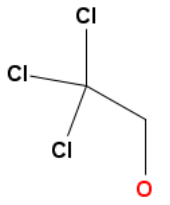


Prediction: Reliability:

Prediction is 56.96 mg/L, but the result shows some critical aspects, which require to be checked:
- only moderately similar compounds with known experimental value in the training set have been found
- accuracy of prediction for similar molecules found in the training set is not optimal
- the maximum error in prediction of similar molecules found in the training set has a moderate value, considering the experimental variability

Compound: Molecule 0
Compound SMILES: O=C(O)C(F)(F)F
Experimental value [-log(mol/l)]: -
Predicted toxicity [-log(mol/l)]: 3.3
Predicted toxicity [mg/l]: 56.96
Molecular Weight: 113.86
Experimental value [mg/l]: -
Reliability: the predicted compound could be out of the Applicability Domain of the model
Remarks:
none

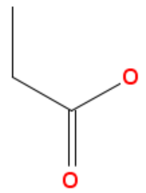
3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



Compound #1

CAS: 115-20-8
Dataset id: 132 (Training set)
SMILES: OCC(Cl)(Cl)Cl
Similarity: 0.718

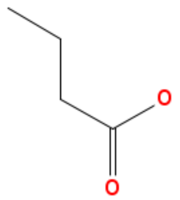
Experimental value [-log(mol/l)]: 3
Predicted value [-log(mol/l)]: 4.046



Compound #2

CAS: 79-09-4
Dataset id: 38 (Training set)
SMILES: O=C(O)CC
Similarity: 0.702

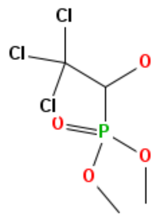
Experimental value [-log(mol/l)]: 3.17
Predicted value [-log(mol/l)]: 2.302



Compound #3

CAS: 107-92-6
Dataset id: 299 (Test set)
SMILES: O=C(O)CCC
Similarity: 0.672

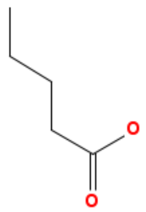
Experimental value [-log(mol/l)]: 3.16
Predicted value [-log(mol/l)]: 2.69



Compound #4

CAS: 52-68-6
Dataset id: 2 (Training set)
SMILES: O=P(OC)(OC)C(O)C(Cl)(Cl)Cl
Similarity: 0.657

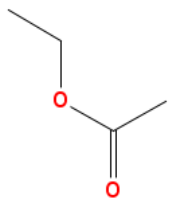
Experimental value [-log(mol/l)]: 9.09
Predicted value [-log(mol/l)]: 6.274



Compound #5

CAS: 109-52-4
Dataset id: 122 (Training set)
SMILES: O=C(O)CCCC
Similarity: 0.649

Experimental value [-log(mol/l)]: 3.36
Predicted value [-log(mol/l)]: 2.959



Compound #6

CAS: 141-78-6
Dataset id: 159 (Training set)
SMILES: O=C(OCC)C
Similarity: 0.638

Experimental value [-log(mol/l)]: 2.08
Predicted value [-log(mol/l)]: 2.607

3.2 Applicability Domain:
Measured Applicability Domain Scores

Global AD Index
AD index = 0.85
Explanation: the predicted compound could be out of the Applicability Domain of the model.

Similar molecules with known experimental value
Similarity index = 0.71
Explanation: only moderately similar compounds with known experimental value in the training set have been found.

Accuracy of prediction for similar molecules
Accuracy index = 0.957
Explanation: accuracy of prediction for similar molecules found in the training set is not optimal.

Concordance for similar molecules
Concordance index = 0.216
Explanation: similar molecules found in the training set have experimental values that agree with the predicted value.

Maximum error of prediction among similar molecules
Max error index = 1.046
Explanation: the maximum error in prediction of similar molecules found in the training set has a moderate value, considering the experimental variability.

Model's descriptors range check
Descriptors range check = True
Explanation: descriptors for this compound have values inside the descriptor range of the compounds of the training set.

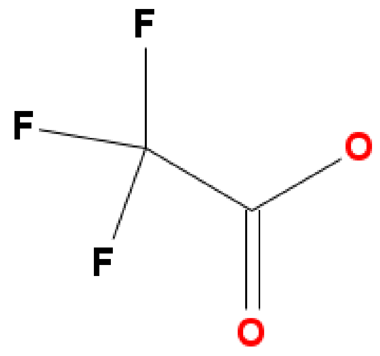
Atom Centered Fragments similarity check
ACF index = 1
Explanation: all atom centered fragment of the compound have been found in the compounds of the training set.

Symbols explanation:

The feature has a good assessment, model is reliable regarding this aspect.
The feature has a non optimal assessment, this aspect should be reviewed by an expert.
The feature has a bad assessment, model is not reliable regarding this aspect.

1. Prediction Summary

Prediction for compound Molecule 0

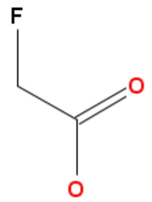


Prediction: Reliability:

Prediction is 180.87 mg/L, but the result shows some critical aspects, which require to be checked:

Compound: Molecule 0
Compound SMILES: O=C(O)C(F)(F)F
Experimental value [-log(mol/l)]: -
Predicted toxicity [-log(mol/l)]: 2.8
Predicted toxicity [mg/l]: 180.87
Molecular Weight: 113.86
Experimental value [mg/l]: -
Reliability: the predicted compound could be out of the Applicability Domain of the model
Remarks:
none

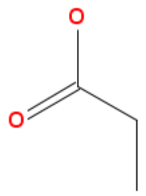
3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



Compound #1

CAS: 144-49-0
Dataset id: 230 (Test set)
SMILES: OC(=O)CF
Similarity: 0.855

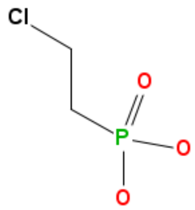
Experimental value [-log(mol/l)]: 2.31
Predicted value [-log(mol/l)]: 2.876



Compound #2

CAS: 79-09-4
Dataset id: 269 (Training set)
SMILES: CCC(O)=O
Similarity: 0.702

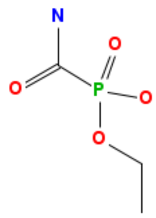
Experimental value [-log(mol/l)]: 3.65
Predicted value [-log(mol/l)]: 3.033



Compound #3

CAS: 16672-87-0
Dataset id: 373 (Training set)
SMILES: OP(O)(=O)CCCl
Similarity: 0.635

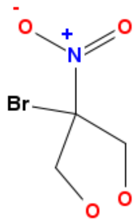
Experimental value [-log(mol/l)]: 3.84
Predicted value [-log(mol/l)]: 3.329



Compound #4

CAS: 59682-52-9
Dataset id: 140 (Training set)
SMILES: CCOP(O)(=O)C(N)=O
Similarity: 0.634

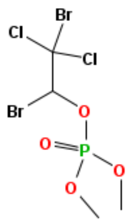
Experimental value [-log(mol/l)]: 1.79
Predicted value [-log(mol/l)]: 3.863



Compound #5

CAS: 52-51-7
Dataset id: 39 (Training set)
SMILES: OCC(Br)(CO)[N+]([O-])=O
Similarity: 0.633

Experimental value [-log(mol/l)]: 5.69
Predicted value [-log(mol/l)]: 4.511



Compound #6

CAS: 300-76-5
Dataset id: 177 (Training set)
SMILES: COP(=O)(OC)OC(Br)C(Cl)(Cl)Br
Similarity: 0.626

Experimental value [-log(mol/l)]: 10.65
Predicted value [-log(mol/l)]: 9.338

3.2 Applicability Domain:
Measured Applicability Domain Scores

Global AD Index
AD index = 0.8
Explanation: the predicted compound could be out of the Applicability Domain of the model.

Similar molecules with known experimental value
Similarity index = 0.76
Explanation: strongly similar compounds with known experimental value in the training set have been found.

Accuracy of prediction for similar molecules
Accuracy index = 0.591
Explanation: accuracy of prediction for similar molecules found in the training set is good.

Concordance for similar molecules
Concordance index = 0.67
Explanation: similar molecules found in the training set have experimental values that agree with the predicted value.

Maximum error of prediction among similar molecules
Max error index = 0.617
Explanation: the maximum error in prediction of similar molecules found in the training set has a low value, considering the experimental variability.

Model's descriptors range check
Descriptors range check = True
Explanation: descriptors for this compound have values inside the descriptor range of the compounds of the training set.

Atom Centered Fragments similarity check
ACF index = 1
Explanation: all atom centered fragment of the compound have been found in the compounds of the training set.

Symbols explanation:

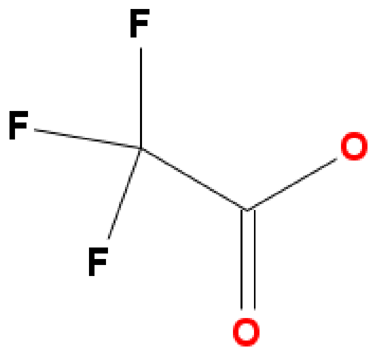
The feature has a good assessment, model is reliable regarding this aspect.

The feature has a non optimal assessment, this aspect should be reviewed by an expert.

The feature has a bad assessment, model is not reliable regarding this aspect.

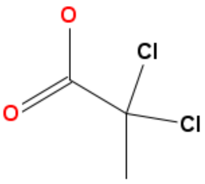
1. Prediction Summary

Prediction for compound Molecule 0

	Prediction: Reliability: **Prediction is N/A, it is not possible to perform an assessment.**

Compound: Molecule 0
Compound SMILES: O=C(O)C(F)(F)F
Experimental value: -
Predicted Toxicity activity: Non Predicted
Molecules used for prediction: 0
Reliability: -
Remarks:
[Model] Unable to perform Applicability Domain check

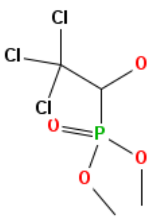
3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



Compound #1

CAS: 127-20-8
Dataset id: 222 (Training set)
SMILES: CC(Cl)(Cl)C(O)=O
Similarity: 0.747

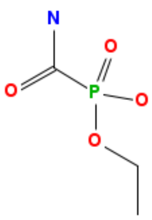
Experimental value: Moderate toxicity (between 1 and 100 µg/bee)
Predicted value: -



Compound #2

CAS: 52-68-6
Dataset id: 79 (Training set)
SMILES: COP(=O)(OC)C(O)C(Cl)(Cl)Cl
Similarity: 0.657

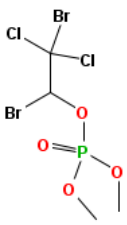
Experimental value: Moderate toxicity (between 1 and 100 µg/bee)
Predicted value: Strong toxicity (lower than 1 µg/bee)



Compound #3

CAS: 25954-13-6
Dataset id: 176 (Training set)
SMILES: CCOP(O)(=O)C(N)=O
Similarity: 0.634

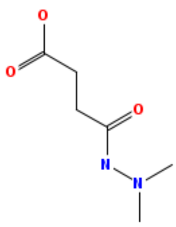
Experimental value: Low toxicity (over 100 µg/bee)
Predicted value: Moderate toxicity (between 1 and 100 µg/bee)



Compound #4

CAS: 300-76-5
Dataset id: 213 (Training set)
SMILES: COP(=O)(OC)OC(Br)C(Cl)(Cl)Br
Similarity: 0.626

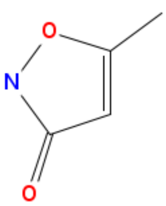
Experimental value: Strong toxicity (lower than 1 µg/bee)
Predicted value: Moderate toxicity (between 1 and 100 µg/bee)



Compound #5

CAS: 1596-84-5
Dataset id: 230 (Training set)
SMILES: CN(C)NC(=O)CCC(O)=O
Similarity: 0.619

Experimental value: Low toxicity (over 100 µg/bee)
Predicted value: Low toxicity (over 100 µg/bee)



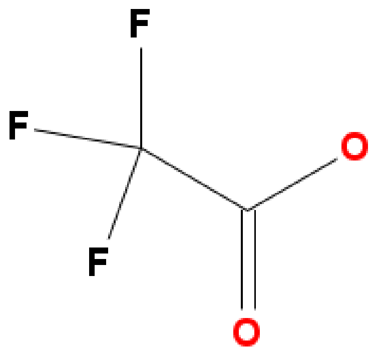
Compound #6

CAS: 10004-44-1
Dataset id: 131 (Training set)
SMILES: CC1=CC(=O)NO1
Similarity: 0.605

Experimental value: Low toxicity (over 100 µg/bee)
Predicted value: -

1. Prediction Summary

Prediction for compound Molecule 0



Prediction:

Reliability:

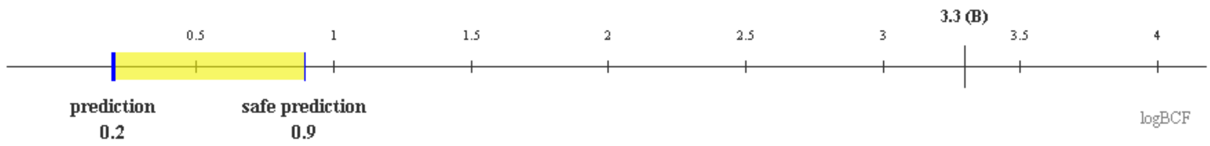
Prediction is 0.2 log(L/kg), but the result shows some critical aspects, which require to be checked:
- only moderately similar compounds with known experimental value in the training set have been found
The following relevant fragments have been found: Carbonyl residue (SR 02); COOH group (PG 01)

Compound: Molecule 0
Compound SMILES: O=C(O)C(F)(F)F
Experimental value [log(L/kg)]: -
Predicted BCF [log(L/kg)]: 0.2
Predicted BCF [L/kg]: 2
Predicted BCF from sub-model 1 (HM) [log(L/kg)]: 0.28
Predicted BCF from sub-model 2 (GA) [log(L/kg)]: 0.4
Predicted LogP (MLogP): 0.37
Structural alerts: Carbonyl residue (SR 02); COOH group (PG 01)
Reliability: the predicted compound could be out of the Applicability Domain of the model
Remarks:
none

2. Possible Use and Uncertainty

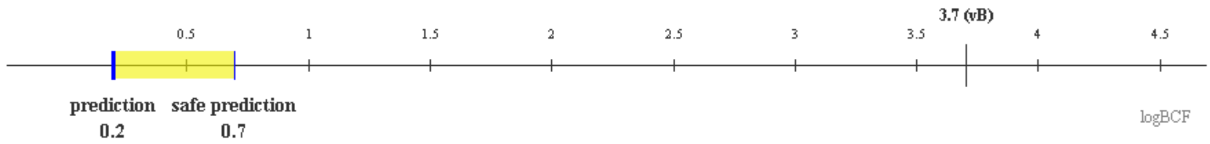
Threshold 3.3 (bioaccumulative)

Following, a chart showing the predicted value together with its conservative confidence interval for safe classification. For the threshold logBCF = 3.3, the current compound can be associated (due to its Applicability Domain index value) to a conservative interval of 0.7 log units.
On this basis, the compound can be safely classified as not bioaccumulative.

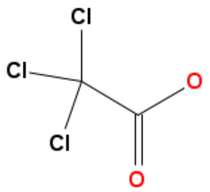


Threshold 3.7 (very bioaccumulative)

Following, a chart showing the predicted value together with its conservative confidence interval for safe classification. For the threshold logBCF = 3.7, the current compound can be associated (due to its Applicability Domain index value) to a conservative interval of 0.5 log units.
On this basis, the compound can be safely classified as not very bioaccumulative.



3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values

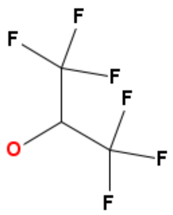


Compound #1

CAS: 76-03-9
Dataset id: 397 (Test set)
SMILES: O=C(O)C(Cl)(Cl)Cl
Similarity: 0.844

Experimental value [log(L/kg)]: -0.15
Predicted value [log(L/kg)]: -0.038

Alerts (found also in the target): Carbonyl residue (SR 02); COOH group (PG 01)

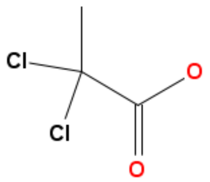


Compound #2

CAS: 920-66-1
Dataset id: 263 (Training set)
SMILES: FC(F)(F)C(O)C(F)(F)F
Similarity: 0.81

Experimental value [log(L/kg)]: 0.3
Predicted value [log(L/kg)]: 0.601

Alerts (not found in the target): OH group (PG 06)

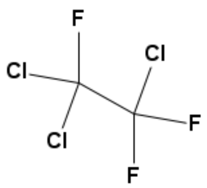


Compound #3

CAS: 75-99-0
Dataset id: 468 (Test set)
SMILES: O=C(O)C(C)(Cl)Cl
Similarity: 0.747

Experimental value [log(L/kg)]: 0.85
Predicted value [log(L/kg)]: 0.075

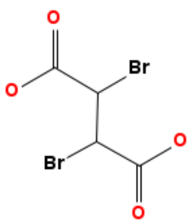
Alerts (found also in the target): Carbonyl residue (SR 02); COOH group (PG 01)



Compound #4

CAS: 76-13-1
Dataset id: 257 (Training set)
SMILES: FC(F)(C(F)(Cl)Cl)Cl
Similarity: 0.699

Experimental value [log(L/kg)]: 1.7
Predicted value [log(L/kg)]: 1.387



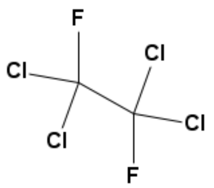
Compound #5

CAS: 526-78-3
Dataset id: 71 (Training set)
SMILES: O=C(O)C(C(C(=O)O)Br)Br
Similarity: 0.685

Experimental value [log(L/kg)]: 0.81
Predicted value [log(L/kg)]: 0.227

Alerts (found also in the target): Carbonyl residue (SR 02); COOH group (PG 01)

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



Compound #6

CAS: 76-12-0
Dataset id: 258 (Test set)
SMILES: FC(C(F)(Cl)Cl)(Cl)Cl
Similarity: 0.661

Experimental value [log(L/kg)]: 1.78
Predicted value [log(L/kg)]: 1.29

3.2 Applicability Domain:
Measured Applicability Domain Scores

Global AD Index
AD index = 0.85
Explanation: the predicted compound could be out of the Applicability Domain of the model.

Similar molecules with known experimental value
Similarity index = 0.826
Explanation: only moderately similar compounds with known experimental value in the training set have been found.

Accuracy of prediction for similar molecules
Accuracy index = 0.206
Explanation: accuracy of prediction for similar molecules found in the training set is good.

Concordance for similar molecules
Concordance index = 0.225
Explanation: similar molecules found in the training set have experimental values that agree with the predicted value.

Maximum error of prediction among similar molecules
Max error index = 0.301
Explanation: the maximum error in prediction of similar molecules found in the training set has a low value, considering the experimental variability.

Model's descriptors range check
Descriptors range check = True
Explanation: descriptors for this compound have values inside the descriptor range of the compounds of the training set.

Atom Centered Fragments similarity check
ACF index = 1
Explanation: all atom centered fragment of the compound have been found in the compounds of the training set.

Symbols explanation:

The feature has a good assessment, model is reliable regarding this aspect.
The feature has a non optimal assessment, this aspect should be reviewed by an expert.
The feature has a bad assessment, model is not reliable regarding this aspect.

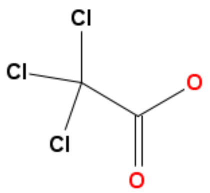
4.1 Reasoning:
Relevant Chemical Fragments and Moieties

(Molecule 0) Reasoning on fragments/structural alerts - 1 of 2:

Fragment found: Carbonyl residue (SR 02)

This chemical contains a carbonyl residue. This residue has been found to be present in a very large (112) number of non-bioaccumulative compounds, even when the logP value was higher than 3.

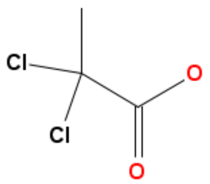
Following, the most similar compounds from the model's dataset having the same fragment.



CAS: 76-03-9
Dataset id: 397 (Test set)
SMILES: O=C(O)C(Cl)(Cl)Cl
Similarity: 0.844

Experimental value [log(L/kg)]: -0.15
Predicted value [log(L/kg)]: -0.038

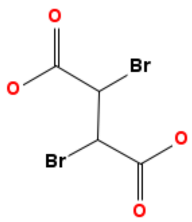
Alerts (found also in the target): Carbonyl residue (SR 02); COOH group (PG 01)



CAS: 75-99-0
Dataset id: 468 (Test set)
SMILES: O=C(O)C(C)(Cl)Cl
Similarity: 0.747

Experimental value [log(L/kg)]: 0.85
Predicted value [log(L/kg)]: 0.075

Alerts (found also in the target): Carbonyl residue (SR 02); COOH group (PG 01)



CAS: 526-78-3
Dataset id: 71 (Training set)
SMILES: O=C(O)C(C(C(=O)O)Br)Br
Similarity: 0.685

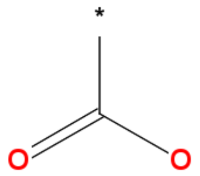
Experimental value [log(L/kg)]: 0.81
Predicted value [log(L/kg)]: 0.227

Alerts (found also in the target): Carbonyl residue (SR 02); COOH group (PG 01)

4.1 Reasoning:
Relevant Chemical Fragments and Moieties

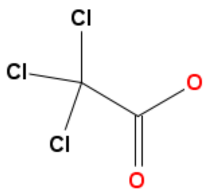
(Molecule 0) Reasoning on fragments/structural alerts - 2 of 2:

Fragment found: COOH group (PG 01)



This chemical contains a COOH polar group. The presence of polar groups increases hydrophilicity, related to lower values of BCF.

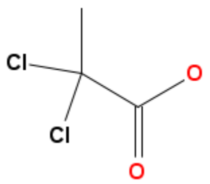
Following, the most similar compounds from the model's dataset having the same fragment.



CAS: 76-03-9
Dataset id: 397 (Test set)
SMILES: O=C(O)C(Cl)(Cl)Cl
Similarity: 0.844

Experimental value [log(L/kg)]: -0.15
Predicted value [log(L/kg)]: -0.038

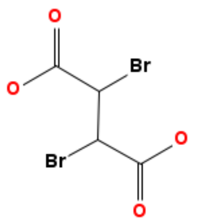
Alerts (found also in the target): Carbonyl residue (SR 02); COOH group (PG 01)



CAS: 75-99-0
Dataset id: 468 (Test set)
SMILES: O=C(O)C(C)(Cl)Cl
Similarity: 0.747

Experimental value [log(L/kg)]: 0.85
Predicted value [log(L/kg)]: 0.075

Alerts (found also in the target): Carbonyl residue (SR 02); COOH group (PG 01)



CAS: 526-78-3
Dataset id: 71 (Training set)
SMILES: O=C(O)C(C(C(=O)O)Br)Br
Similarity: 0.685

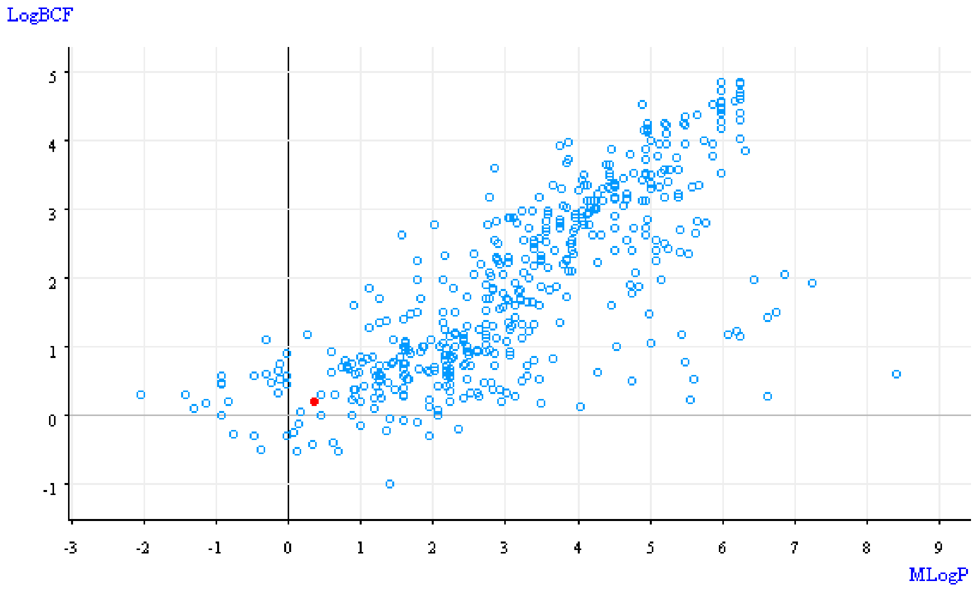
Experimental value [log(L/kg)]: 0.81
Predicted value [log(L/kg)]: 0.227

Alerts (found also in the target): Carbonyl residue (SR 02); COOH group (PG 01)

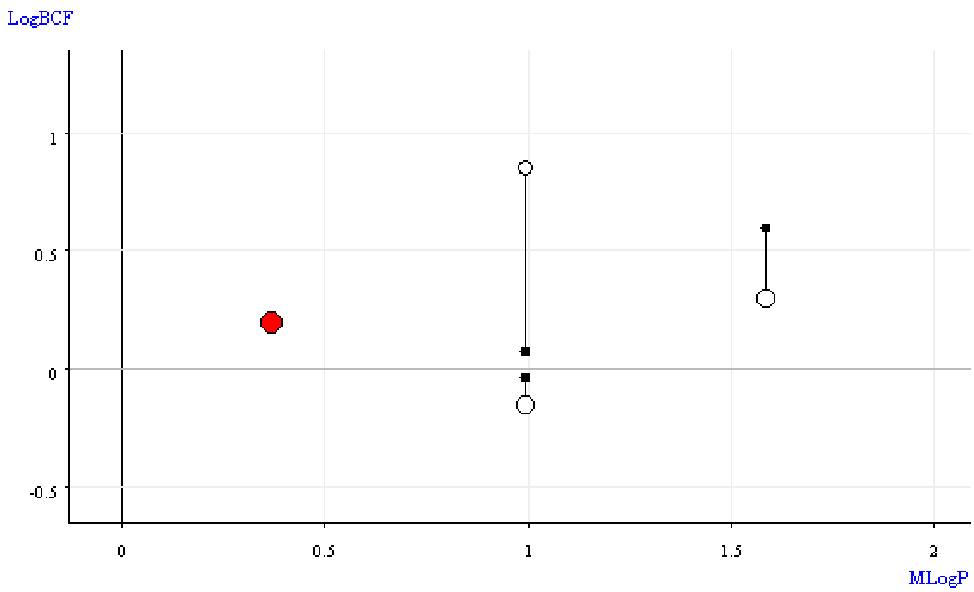
4.2 Reasoning:
Analysis of Molecular Descriptors

Descriptor name: MLogP
Description: LogP is directly correlated to the logBCF value.

Following, a scatterplot of MLogP against response values; experimental values are reported for the training set, predicted value for the studied compound. Light blue dots represent values of compounds from training set, red dot is the value of the studied compound.

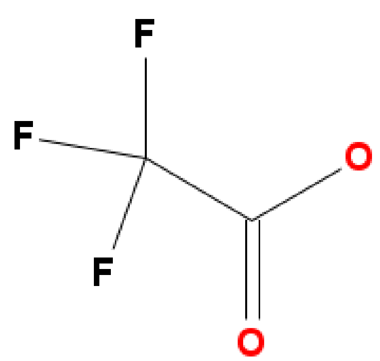


Following, a scatterplot of MLogP against response values only for 3 most similar compounds in the training set. Red dot is the value of the studied compound, black outlined circles represents experimental values of compounds from training set, black dots represents predicted value of the same compound; the size of the circle is proportional to the similarity to the studied compound.



1. Prediction Summary

Prediction for compound Molecule 0

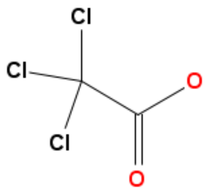


Prediction: Reliability:

Prediction is 0.5 log(L/kg), but the result may be not reliable. A check of the information given in the following section should be done, paying particular attention to the following issues:
- only moderately similar compounds with known experimental value in the training set have been found
- some atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (1 infrequent fragments found)

Compound: Molecule 0
Compound SMILES: O=C(O)C(F)(F)F
Experimental value [log(L/kg)]: -
Predicted BCF [log(L/kg)]: 0.5
Predicted BCF [L/kg]: 3
Predicted LogP (Meylan/Kowwin): 0.5
Predicted LogP reliability: Good
MW: 113.86
Ionic compound: yes
Reliability: the predicted compound is outside the Applicability Domain of the model
Remarks:
none

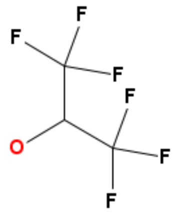
3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



Compound #1

CAS: 76-03-9
Dataset id: 5 (Training set)
SMILES: O=C(O)C(Cl)(Cl)Cl
Similarity: 0.844

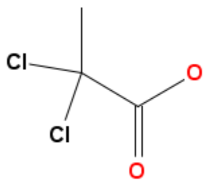
Experimental value [log(L/kg)]: 0.23
Predicted value [log(L/kg)]: 0.5



Compound #2

CAS: 920-66-1
Dataset id: 117 (Training set)
SMILES: FC(F)(F)C(O)C(F)(F)F
Similarity: 0.81

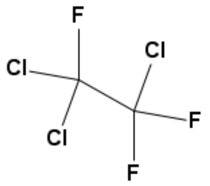
Experimental value [log(L/kg)]: 0.4
Predicted value [log(L/kg)]: 0.762



Compound #3

CAS: 127-20-8
Dataset id: 20 (Training set)
SMILES: O=C(O)C(C)(Cl)Cl
Similarity: 0.747

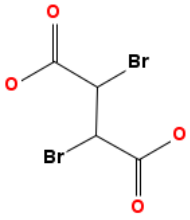
Experimental value [log(L/kg)]: 0.86
Predicted value [log(L/kg)]: 0.5



Compound #4

CAS: 76-13-1
Dataset id: 668 (Test set)
SMILES: FC(F)(C(F)(Cl)Cl)Cl
Similarity: 0.699

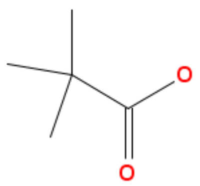
Experimental value [log(L/kg)]: 1.7
Predicted value [log(L/kg)]: 1.752



Compound #5

CAS: 526-78-3
Dataset id: 27 (Training set)
SMILES: O=C(O)C(C(C(=O)O)Br)Br
Similarity: 0.685

Experimental value [log(L/kg)]: 0.81
Predicted value [log(L/kg)]: 0.5



Compound #6

CAS: 75-98-9
Dataset id: 4 (Training set)
SMILES: O=C(O)C(C)(C)C
Similarity: 0.67

Experimental value [log(L/kg)]: 0.36
Predicted value [log(L/kg)]: 0.5

3.2 Applicability Domain:
Measured Applicability Domain Scores

Global AD Index
AD index = 0.702
Explanation: the predicted compound is outside the Applicability Domain of the model.

Similar molecules with known experimental value
Similarity index = 0.826
Explanation: only moderately similar compounds with known experimental value in the training set have been found.

Accuracy of prediction for similar molecules
Accuracy index = 0.316
Explanation: accuracy of prediction for similar molecules found in the training set is good.

Concordance for similar molecules
Concordance index = 0.185
Explanation: similar molecules found in the training set have experimental values that agree with the predicted value.

Maximum error of prediction among similar molecules
Max error index = 0.362
Explanation: the maximum error in prediction of similar molecules found in the training set has a low value, considering the experimental variability.

Reliability of logP prediction
LogP reliability = 1
Explanation: reliability of logP value used by the model is good.

Model's descriptors range check
Descriptors range check = True
Explanation: descriptors for this compound have values inside the defined range.

Atom Centered Fragments similarity check
ACF index = 0.85
Explanation: some atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (1 infrequent fragments found).

Symbols explanation:

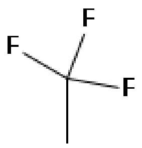
The feature has a good assessment, model is reliable regarding this aspect.

The feature has a non optimal assessment, this aspect should be reviewed by an expert.

The feature has a bad assessment, model is not reliable regarding this aspect.

4.1 Reasoning:
Relevant Chemical Fragments and Moieties

(Molecule 0) Reasoning on rare and missing Atom Centered Fragments.
The following Atom Centered Fragments have been found in the molecule, but they are not found or rarely found in the model's training set:

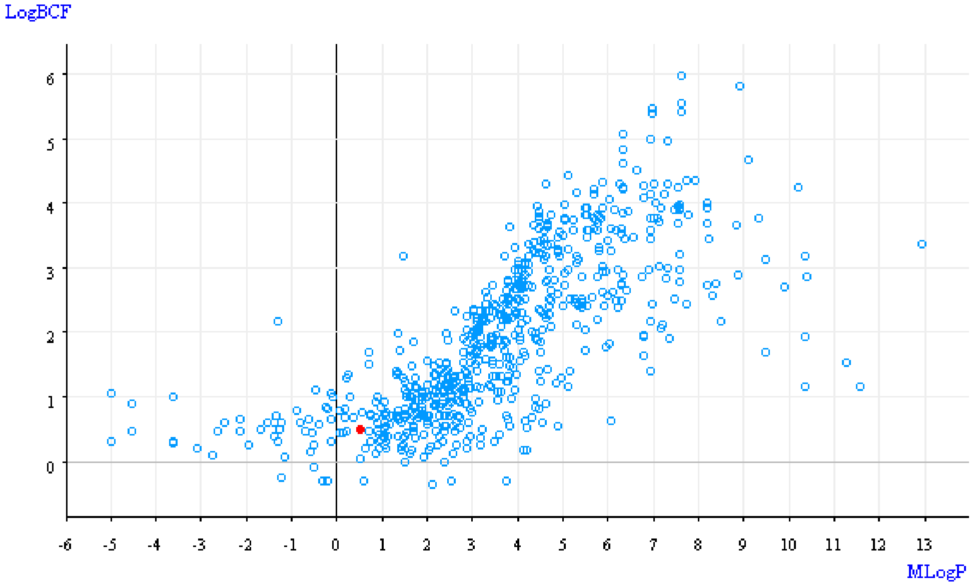


Fragment defined by the SMILES: FC(F)(F)C
The fragment has less than 3 occurrences in the model's training set

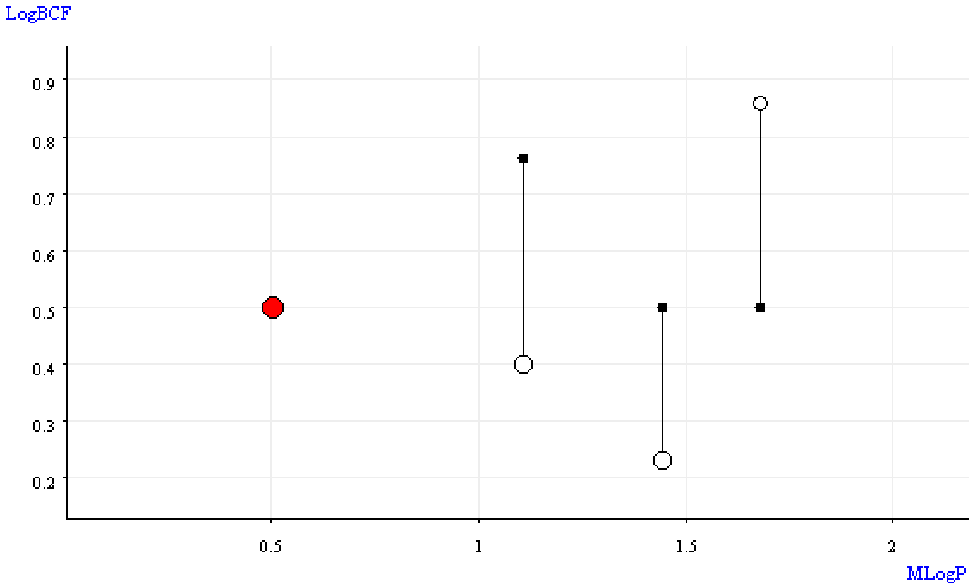
4.2 Reasoning:
Analysis of Molecular Descriptors

Descriptor name: MLogP
Description: LogP is directly correlated to the logBCF value.

Following, a scatterplot of MLogP against response values; experimental values are reported for the training set, predicted value for the studied compound. Light blue dots represent values of compounds from training set, red dot is the value of the studied compound.

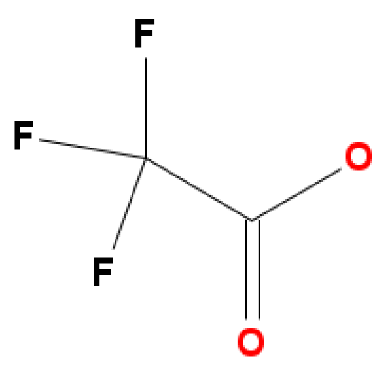


Following, a scatterplot of MLogP against response values only for 3 most similar compounds in the training set. Red dot is the value of the studied compound, black outlined circles represents experimental values of compounds from training set, black dots represents predicted value of the same compound; the size of the circle is proportional to the similarity to the studied compound.



1. Prediction Summary

Prediction for compound Molecule 0



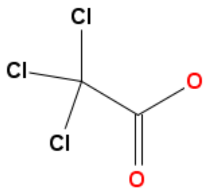
Prediction:

Reliability:

Prediction is 0.27 log(L/kg), but the result may be not reliable. A check of the information given in the following section should be done, paying particular attention to the following issues:
- accuracy of prediction for similar molecules found in the training set is not optimal
- the maximum error in prediction of similar molecules found in the training set has a high value, considering the experimental variability

Compound: Molecule 0
Compound SMILES: O=C(O)C(F)(F)F
Experimental value [log(L/kg)]: -
Predicted BCF [log(L/kg)]: 0.27
Molecules used for prediction: 3
Reliability: the predicted compound is outside the Applicability Domain of the model
Remarks:
none

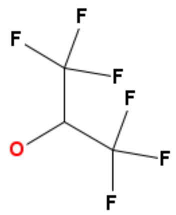
3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



Compound #1

CAS: 76-03-9
Dataset id: 41 (Training set)
SMILES: O=C(O)C(Cl)(Cl)Cl
Similarity: 0.844

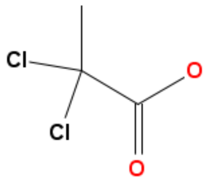
Experimental value [log(L/kg)]: 0.025
Predicted value [log(L/kg)]: 0.409



Compound #2

CAS: 920-66-1
Dataset id: 391 (Training set)
SMILES: FC(F)(F)C(O)C(F)(F)F
Similarity: 0.81

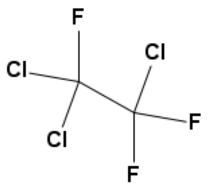
Experimental value [log(L/kg)]: 0.244
Predicted value [log(L/kg)]: 1.753



Compound #3

CAS: 75-99-0
Dataset id: 40 (Training set)
SMILES: O=C(O)C(C)(Cl)Cl
Similarity: 0.747

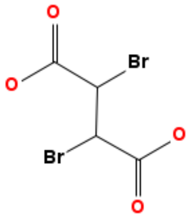
Experimental value [log(L/kg)]: 0.664
Predicted value [log(L/kg)]: 0.188



Compound #4

CAS: 76-13-1
Dataset id: 43 (Training set)
SMILES: FC(F)(C(F)(Cl)Cl)Cl
Similarity: 0.699

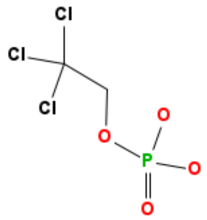
Experimental value [log(L/kg)]: 1.623
Predicted value [log(L/kg)]: 1.464



Compound #5

CAS: 526-78-3
Dataset id: 325 (Training set)
SMILES: O=C(O)C(C(C(=O)O)Br)Br
Similarity: 0.685

Experimental value [log(L/kg)]: 0.43
Predicted value [log(L/kg)]: 0.02



Compound #6

CAS: 306-52-5
Dataset id: 302 (Training set)
SMILES: O=P(O)(O)OCC(Cl)(Cl)Cl
Similarity: 0.682

Experimental value [log(L/kg)]: 0.078
Predicted value [log(L/kg)]: -0.074

3.2 Applicability Domain:
Measured Applicability Domain Scores

Global AD Index
AD index = 0.7
Explanation: the predicted compound is outside the Applicability Domain of the model.

Similar molecules with known experimental value
Similarity index = 0.793
Explanation: strongly similar compounds with known experimental value in the training set have been found.

Accuracy of prediction for similar molecules
Accuracy index = 0.789
Explanation: accuracy of prediction for similar molecules found in the training set is not optimal.

Concordance for similar molecules
Concordance index = 0.222
Explanation: similar molecules found in the training set have experimental values that agree with the predicted value.

Maximum error of prediction among similar molecules
Max error index = 1.509
Explanation: the maximum error in prediction of similar molecules found in the training set has a high value, considering the experimental variability.

Atom Centered Fragments similarity check
ACF index = 1
Explanation: all atom centered fragment of the compound have been found in the compounds of the training set.

Symbols explanation:

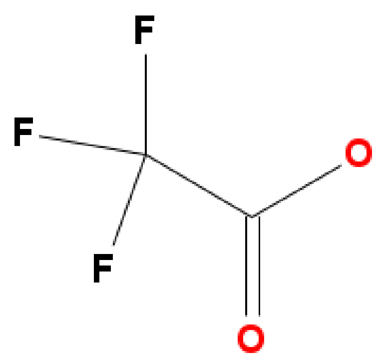
The feature has a good assessment, model is reliable regarding this aspect.

The feature has a non optimal assessment, this aspect should be reviewed by an expert.

The feature has a bad assessment, model is not reliable regarding this aspect.

1. Prediction Summary

Prediction for compound Molecule 0

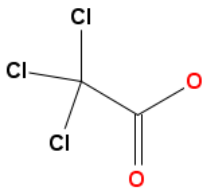


Prediction: Reliability:

Prediction is NON Readily Biodegradable, but the result shows some critical aspects, which require to be checked:
- only moderately similar compounds with known experimental value in the training set have been found
- some similar molecules found in the training set have experimental values that disagree with the predicted value
- some atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (1 infrequent fragments found)
The following relevant fragments have been found: Non RB alert no. 11 (fluorine); Possible RB alert no. 14 (acetaldehyde)

Compound: Molecule 0
Compound SMILES: O=C(O)C(F)(F)F
Experimental value: -
Predicted RB activity: NON Readily Biodegradable
No. alerts for non RB: 1
No. alerts for possible non RB: 0
No. alerts for RB: 0
No. alerts for possible RB: 1
Structural alerts: Non RB alert no. 11 (fluorine); Possible RB alert no. 14 (acetaldehyde)
Reliability: the predicted compound could be out of the Applicability Domain of the model
Remarks:
none

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



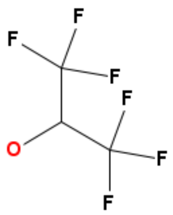
Compound #1

CAS: 76-03-9
Dataset id: 32 (Training set)
SMILES: O=C(O)C(Cl)(Cl)Cl
Similarity: 0.844

Experimental value: NON Readily Biodegradable
Predicted value: NON Readily Biodegradable

Alerts (found also in the target): Possible RB alert no. 14 (acetaldehyde)

Alerts (not found in the target): Non RB alert no. 32 (1,1,1-trichloroethane)

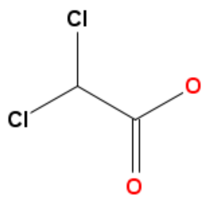


Compound #2

CAS: 920-66-1
Dataset id: 284 (Test set)
SMILES: FC(F)(F)C(O)C(F)(F)F
Similarity: 0.81

Experimental value: NON Readily Biodegradable
Predicted value: NON Readily Biodegradable

Alerts (found also in the target): Non RB alert no. 11 (fluorine)

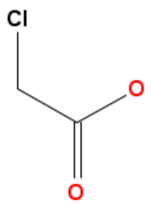


Compound #3

CAS: 79-43-6
Dataset id: 52 (Test set)
SMILES: O=C(O)C(Cl)Cl
Similarity: 0.795

Experimental value: Readily Biodegradable
Predicted value: Possible Readily Biodegradable

Alerts (found also in the target): Possible RB alert no. 14 (acetaldehyde)

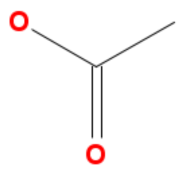


Compound #4

CAS: 79-11-8
Dataset id: 50 (Training set)
SMILES: O=C(O)CCl
Similarity: 0.761

Experimental value: Readily Biodegradable
Predicted value: Possible Readily Biodegradable

Alerts (found also in the target): Possible RB alert no. 14 (acetaldehyde)



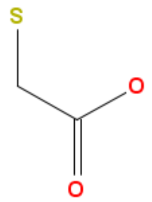
Compound #5

CAS: 64-19-7
Dataset id: 414 (Training set)
SMILES: O=C(O)C
Similarity: 0.739

Experimental value: Readily Biodegradable
Predicted value: Possible Readily Biodegradable

Alerts (found also in the target): Possible RB alert no. 14 (acetaldehyde)

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



Compound #6

CAS: 68-11-1
Dataset id: 16 (Training set)
SMILES: O=C(O)CS
Similarity: 0.72

Experimental value: Readily Biodegradable
Predicted value: Possible Readily Biodegradable

Alerts (found also in the target): Possible RB alert no. 14 (acetaldehyde)

3.2 Applicability Domain:
Measured Applicability Domain Scores

⚠	**Global AD Index** AD index = 0.696 Explanation: the predicted compound could be out of the Applicability Domain of the model.
⚠	**Similar molecules with known experimental value** Similarity index = 0.814 Explanation: only moderately similar compounds with known experimental value in the training set have been found.
✔	**Accuracy of prediction for similar molecules** Accuracy index = 1 Explanation: accuracy of prediction for similar molecules found in the training set is good.
⚠	**Concordance for similar molecules** Concordance index = 0.678 Explanation: some similar molecules found in the training set have experimental values that disagree with the predicted value.
⚠	**Atom Centered Fragments similarity check** ACF index = 0.85 Explanation: some atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (1 infrequent fragments found).

Symbols explanation:

✔ The feature has a good assessment, model is reliable regarding this aspect.

⚠ The feature has a non optimal assessment, this aspect should be reviewed by an expert.

✖ The feature has a bad assessment, model is not reliable regarding this aspect.

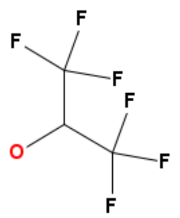
4.1 Reasoning:
Relevant Chemical Fragments and Moieties

(Molecule 0) Reasoning on fragments/structural alerts - 1 of 2:

Fragment found: Non RB alert no. 11 (fluorine)

Structural alert related to non ready biodegradability activity, defined by the SMARTS: F.

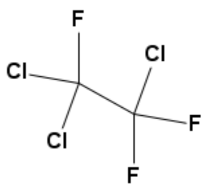
Following, the most similar compounds from the model's dataset having the same fragment.



CAS: 920-66-1
Dataset id: 284 (Test set)
SMILES: FC(F)(F)C(O)C(F)(F)F
Similarity: 0.81

Experimental value: NON Readily Biodegradable
Predicted value: NON Readily Biodegradable

Alerts (found also in the target): Non RB alert no. 11 (fluorine)

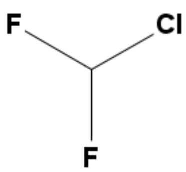


CAS: 76-13-1
Dataset id: 34 (Test set)
SMILES: FC(F)(C(F)(Cl)Cl)Cl
Similarity: 0.699

Experimental value: NON Readily Biodegradable
Predicted value: NON Readily Biodegradable

Alerts (found also in the target): Non RB alert no. 11 (fluorine)

Alerts (not found in the target): Non RB alert no. 3 (1,2-dichloroethane)



CAS: 75-45-6
Dataset id: 27 (Training set)
SMILES: FC(F)Cl
Similarity: 0.662

Experimental value: NON Readily Biodegradable
Predicted value: NON Readily Biodegradable

Alerts (found also in the target): Non RB alert no. 11 (fluorine)

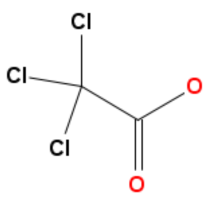
4.1 Reasoning:
Relevant Chemical Fragments and Moieties

(Molecule 0) Reasoning on fragments/structural alerts - 2 of 2:

Fragment found: Possible RB alert no. 14 (acetaldehyde)

Structural alert related to possible ready biodegradability activity, defined by the SMARTS: O=CC.

Following, the most similar compounds from the model's dataset having the same fragment.

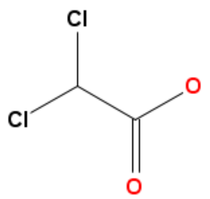


CAS: 76-03-9
Dataset id: 32 (Training set)
SMILES: O=C(O)C(Cl)(Cl)Cl
Similarity: 0.844

Experimental value: NON Readily Biodegradable
Predicted value: NON Readily Biodegradable

Alerts (found also in the target): Possible RB alert no. 14 (acetaldehyde)

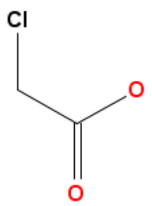
Alerts (not found in the target): Non RB alert no. 32 (1,1,1-trichloroethane)



CAS: 79-43-6
Dataset id: 52 (Test set)
SMILES: O=C(O)C(Cl)Cl
Similarity: 0.795

Experimental value: Readily Biodegradable
Predicted value: Possible Readily Biodegradable

Alerts (found also in the target): Possible RB alert no. 14 (acetaldehyde)



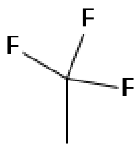
CAS: 79-11-8
Dataset id: 50 (Training set)
SMILES: O=C(O)CCl
Similarity: 0.761

Experimental value: Readily Biodegradable
Predicted value: Possible Readily Biodegradable

Alerts (found also in the target): Possible RB alert no. 14 (acetaldehyde)

4.1 Reasoning:
Relevant Chemical Fragments and Moieties

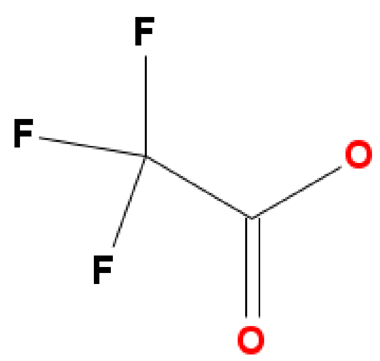
(Molecule 0) Reasoning on rare and missing Atom Centered Fragments.
The following Atom Centered Fragments have been found in the molecule, but they are not found or rarely found in the model's training set:



Fragment defined by the SMILES: FC(F)(F)C
The fragment has less than 3 occurrences in the model's training set

1. Prediction Summary

Prediction for compound Molecule 0



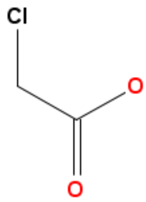
Prediction: Reliability:

Prediction is nP, but the result may be not reliable. A check of the information given in the following section should be done, paying particular attention to the following issues:
- only moderately similar compounds with known experimental value in the training set have been found
- accuracy of prediction for similar molecules found in the training set is not adequate
- similar molecules found in the training set have experimental values that disagree with the predicted value
- KNN model has given no output and prediction has based only on found alerts
- a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (1 unknown fragments and 1 infrequent fragments found)

Compound: Molecule 0
Compound SMILES: O=C(O)C(F)(F)F
Experimental value: -
Predicted persistence in sediment: nP
Molecules used for prediction: 0
Structural alerts: nP (sediment) alert no. 1; nP (sediment) alert no. 4
Reliability: the predicted compound is outside the Applicability Domain of the model
Remarks:
none

3.1 Applicability Domain:

Similar Compounds, with Predicted and Experimental Values



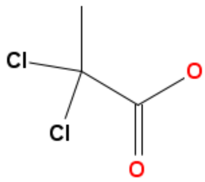
Compound #1

CAS: 79-11-8
Dataset id: 46 (Training set)
SMILES: C(=O)(O)CCl
Similarity: 0.761

Experimental value: nP/P
Predicted value: nP

Alerts (found also in the target): nP (sediment) alert no. 1; nP (sediment) alert no. 4

Alerts (not found in the target): nP (sediment) alert no. 3



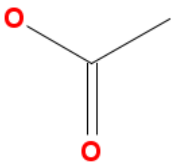
Compound #2

CAS: 75-99-0
Dataset id: 39 (Training set)
SMILES: O=C(O)C(C)(Cl)Cl
Similarity: 0.747

Experimental value: nP/P
Predicted value: nP

Alerts (found also in the target): nP (sediment) alert no. 1; nP (sediment) alert no. 4

Alerts (not found in the target): nP (sediment) alert no. 3

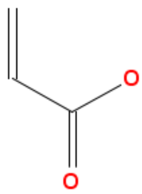


Compound #3

CAS: 64-19-7
Dataset id: 18 (Training set)
SMILES: O=C(O)C
Similarity: 0.739

Experimental value: nP
Predicted value: nP

Alerts (found also in the target): nP (sediment) alert no. 1; nP (sediment) alert no. 4

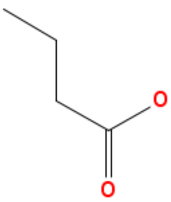


Compound #4

CAS: 79-10-7
Dataset id: 45 (Training set)
SMILES: O=C(O)C=C
Similarity: 0.675

Experimental value: nP
Predicted value: nP

Alerts (found also in the target): nP (sediment) alert no. 1; nP (sediment) alert no. 4



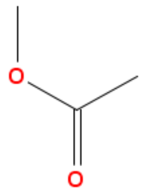
Compound #5

CAS: 107-92-6
Dataset id: 109 (Training set)
SMILES: O=C(O)CCC
Similarity: 0.672

Experimental value: nP
Predicted value: nP

Alerts (found also in the target): nP (sediment) alert no. 1; nP (sediment) alert no. 4

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



Compound #6

CAS: 79-20-9
Dataset id: 47 (Training set)
SMILES: O=C(OC)C
Similarity: 0.664

Experimental value: nP
Predicted value: nP

Alerts (found also in the target): nP (sediment) alert no. 1; nP (sediment) alert no. 4

3.2 Applicability Domain:
Measured Applicability Domain Scores

Global AD Index AD index = 0.215 Explanation: the predicted compound is outside the Applicability Domain of the model.

Similar molecules with known experimental value Similarity index = 0.749 Explanation: only moderately similar compounds with known experimental value in the training set have been found.
Accuracy of prediction for similar molecules Accuracy index = 0.327 Explanation: accuracy of prediction for similar molecules found in the training set is not adequate.
Concordance for similar molecules Concordance index = 0.327 Explanation: similar molecules found in the training set have experimental values that disagree with the predicted value.
Concordance of prediction with found structural alerts Structural alerts concordance = 0.85 Explanation: KNN model has given no output and prediction has based only on found alerts.
Atom Centered Fragments similarity check ACF index = 0.51 Explanation: a prominent number of atom centered fragments of the compound have not been found in the compounds of the training set or are rare fragments (1 unknown fragments and 1 infrequent fragments found).

Symbols explanation:

The feature has a good assessment, model is reliable regarding this aspect.

The feature has a non optimal assessment, this aspect should be reviewed by an expert.

The feature has a bad assessment, model is not reliable regarding this aspect.

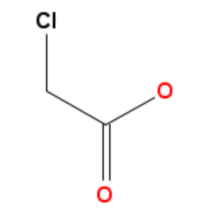
4.1 Reasoning:
Relevant Chemical Fragments and Moieties

(Molecule 0) Reasoning on fragments/structural alerts - 1 of 2:

Fragment found: nP (sediment) alert no. 1

Fragment related to nP compounds (sediment), defined by the SMARTS: O=CC

Following, the most similar compounds from the model's dataset having the same fragment.

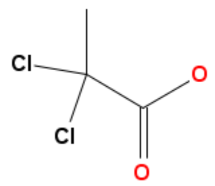


CAS: 79-11-8
Dataset id: 46 (Training set)
SMILES: C(=O)(O)CCl
Similarity: 0.761

Experimental value: nP/P
Predicted value: nP

Alerts (found also in the target): nP (sediment) alert no. 1; nP (sediment) alert no. 4

Alerts (not found in the target): nP (sediment) alert no. 3

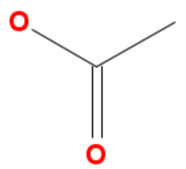


CAS: 75-99-0
Dataset id: 39 (Training set)
SMILES: O=C(O)C(C)(Cl)Cl
Similarity: 0.747

Experimental value: nP/P
Predicted value: nP

Alerts (found also in the target): nP (sediment) alert no. 1; nP (sediment) alert no. 4

Alerts (not found in the target): nP (sediment) alert no. 3



CAS: 64-19-7
Dataset id: 18 (Training set)
SMILES: O=C(O)C
Similarity: 0.739

Experimental value: nP
Predicted value: nP

Alerts (found also in the target): nP (sediment) alert no. 1; nP (sediment) alert no. 4

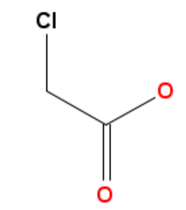
4.1 Reasoning:
Relevant Chemical Fragments and Moieties

(Molecule 0) Reasoning on fragments/structural alerts - 2 of 2:

Fragment found: nP (sediment) alert no. 4

Fragment related to nP compounds (sediment), defined by the SMARTS: OC(C)

Following, the most similar compounds from the model's dataset having the same fragment.

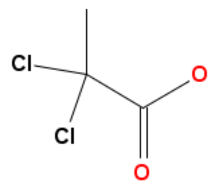


CAS: 79-11-8
Dataset id: 46 (Training set)
SMILES: C(=O)(O)CCl
Similarity: 0.761

Experimental value: nP/P
Predicted value: nP

Alerts (found also in the target): nP (sediment) alert no. 1; nP (sediment) alert no. 4

Alerts (not found in the target): nP (sediment) alert no. 3

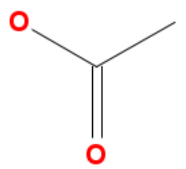


CAS: 75-99-0
Dataset id: 39 (Training set)
SMILES: O=C(O)C(C)(Cl)Cl
Similarity: 0.747

Experimental value: nP/P
Predicted value: nP

Alerts (found also in the target): nP (sediment) alert no. 1; nP (sediment) alert no. 4

Alerts (not found in the target): nP (sediment) alert no. 3



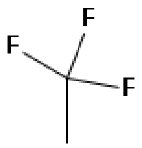
CAS: 64-19-7
Dataset id: 18 (Training set)
SMILES: O=C(O)C
Similarity: 0.739

Experimental value: nP
Predicted value: nP

Alerts (found also in the target): nP (sediment) alert no. 1; nP (sediment) alert no. 4

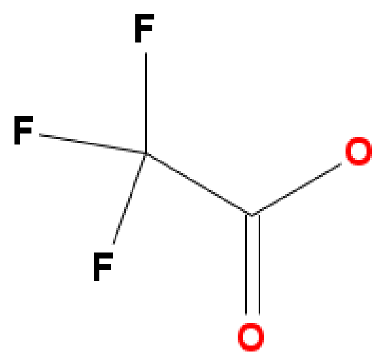
4.1 Reasoning:
Relevant Chemical Fragments and Moieties

(Molecule 0) Reasoning on rare and missing Atom Centered Fragments.
The following Atom Centered Fragments have been found in the molecule, but they are not found or rarely found in the model's training set:

	Fragment defined by the SMILES: FC The fragment has less than 3 occurrences in the model's training set
	Fragment defined by the SMILES: FC(F)(F)C The fragment has never been found in the model's training set

1. Prediction Summary

Prediction for compound Molecule 0

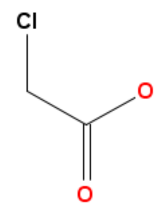


Prediction: ● Reliability: ★ ★ ★

Prediction is nP, the result appears reliable. Anyhow, you should check it through the evaluation of the information given in the following sections. Anyway some issues could be not optimal:
- only moderately similar compounds with known experimental value in the training set have been found

Compound: Molecule 0
Compound SMILES: O=C(O)C(F)(F)F
Experimental value: -
Predicted persistence in soil: nP
Molecules used for prediction: 2
Structural alerts: nP (soil) alert no. 20
Reliability: the predicted compound is into the Applicability Domain of the model
Remarks:
none

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values

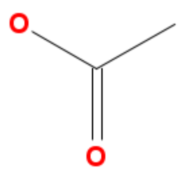


Compound #1

CAS: 79-11-8
Dataset id: 44 (Training set)
SMILES: C(=O)(O)CCl
Similarity: 0.761

Experimental value: nP
Predicted value: nP

Alerts (found also in the target): nP (soil) alert no. 20

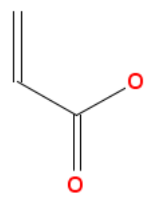


Compound #2

CAS: 64-19-7
Dataset id: 17 (Training set)
SMILES: O=C(O)C
Similarity: 0.739

Experimental value: nP
Predicted value: nP

Alerts (found also in the target): nP (soil) alert no. 20



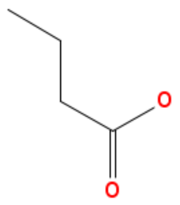
Compound #3

CAS: 79-10-7
Dataset id: 43 (Training set)
SMILES: O=C(O)C=C
Similarity: 0.675

Experimental value: nP
Predicted value: nP

Alerts (found also in the target): nP (soil) alert no. 20

Alerts (not found in the target): nP (soil) alert no. 6

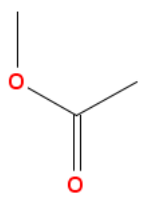


Compound #4

CAS: 107-92-6
Dataset id: 105 (Training set)
SMILES: O=C(O)CCC
Similarity: 0.672

Experimental value: nP
Predicted value: nP

Alerts (found also in the target): nP (soil) alert no. 20



Compound #5

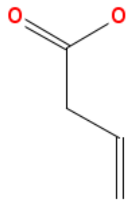
CAS: 79-20-9
Dataset id: 45 (Training set)
SMILES: O=C(OC)C
Similarity: 0.664

Experimental value: nP
Predicted value: nP

Alerts (found also in the target): nP (soil) alert no. 20

Alerts (not found in the target): nP (soil) alert no. 18

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



Compound #6

CAS: 625-38-7
Dataset id: 194 (Training set)
SMILES: C=CCC(=O)O
Similarity: 0.657

Experimental value: nP
Predicted value: nP

Alerts (found also in the target): nP (soil) alert no. 20

3.2 Applicability Domain:
Measured Applicability Domain Scores

Global AD Index
AD index = 0.866
Explanation: the predicted compound is into the Applicability Domain of the model.

Similar molecules with known experimental value
Similarity index = 0.75
Explanation: only moderately similar compounds with known experimental value in the training set have been found.

Accuracy of prediction for similar molecules
Accuracy index = 1
Explanation: accuracy of prediction for similar molecules found in the training set is good.

Concordance for similar molecules
Concordance index = 1
Explanation: similar molecules found in the training set have experimental values that agree with the predicted value.

Concordance of prediction with found structural alerts
Structural alerts concordance = 1
Explanation: all found alerts are related to experimental values in agreement with the prediction.

Atom Centered Fragments similarity check
ACF index = 1
Explanation: all atom centered fragment of the compound have been found in the compounds of the training set.

Symbols explanation:

The feature has a good assessment, model is reliable regarding this aspect.

The feature has a non optimal assessment, this aspect should be reviewed by an expert.

The feature has a bad assessment, model is not reliable regarding this aspect.

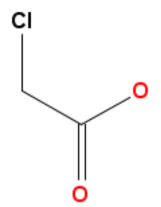
4.1 Reasoning:
Relevant Chemical Fragments and Moieties

(Molecule 0) Reasoning on fragments/structural alerts:

Fragment found: nP (soil) alert no. 20

Chemical class related to nP compounds (soil), defined by the presence of a single carboxylic acid (aliphatic)

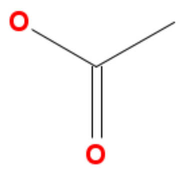
Following, the most similar compounds from the model's dataset having the same fragment.



CAS: 79-11-8
Dataset id: 44 (Training set)
SMILES: C(=O)(O)CCl
Similarity: 0.761

Experimental value: nP
Predicted value: nP

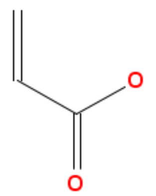
Alerts (found also in the target): nP (soil) alert no. 20



CAS: 64-19-7
Dataset id: 17 (Training set)
SMILES: O=C(O)C
Similarity: 0.739

Experimental value: nP
Predicted value: nP

Alerts (found also in the target): nP (soil) alert no. 20



CAS: 79-10-7
Dataset id: 43 (Training set)
SMILES: O=C(O)C=C
Similarity: 0.675

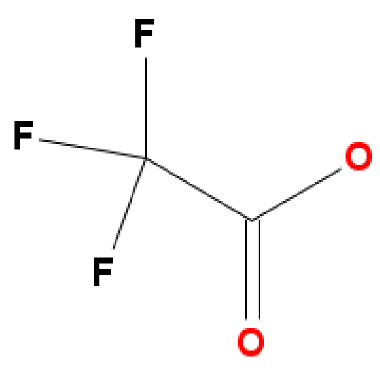
Experimental value: nP
Predicted value: nP

Alerts (found also in the target): nP (soil) alert no. 20

Alerts (not found in the target): nP (soil) alert no. 6

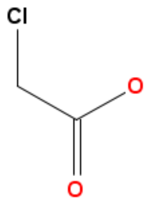
1. Prediction Summary

Prediction for compound Molecule 0

	Prediction: Reliability: **Prediction is nP, but the result shows some critical aspects, which require to be checked:** **- only moderately similar compounds with known experimental value in the training set have been found** **- accuracy of prediction for similar molecules found in the training set is not optimal** **- some similar molecules found in the training set have experimental values that disagree with the predicted value**

Compound: Molecule 0
Compound SMILES: O=C(O)C(F)(F)F
Experimental value: -
Predicted persistence in water: nP
Molecules used for prediction: 3
Structural alerts: nP (sediment) alert no. 1; nP (sediment) alert no. 8; nP (sediment) alert no. 10; nP (sediment) alert no. 13; nP (sediment) alert no. 22
Reliability: the predicted compound could be out of the Applicability Domain of the model
Remarks:
none

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values

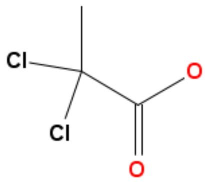


Compound #1

CAS: 79-11-8
Dataset id: 45 (Training set)
SMILES: C(=O)(O)CCl
Similarity: 0.761

Experimental value: nP
Predicted value: nP

Alerts (found also in the target): nP (sediment) alert no. 1; nP (sediment) alert no. 8; nP (sediment) alert no. 10; nP (sediment) alert no. 13; nP (sediment) alert no. 22

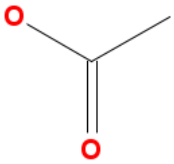


Compound #2

CAS: 75-99-0
Dataset id: 38 (Training set)
SMILES: O=C(O)C(C)(Cl)Cl
Similarity: 0.747

Experimental value: P/vP
Predicted value: nP

Alerts (found also in the target): nP (sediment) alert no. 1; nP (sediment) alert no. 8; nP (sediment) alert no. 10; nP (sediment) alert no. 13; nP (sediment) alert no. 22

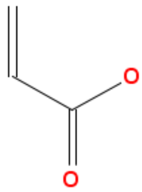


Compound #3

CAS: 64-19-7
Dataset id: 17 (Training set)
SMILES: O=C(O)C
Similarity: 0.739

Experimental value: nP
Predicted value: nP

Alerts (found also in the target): nP (sediment) alert no. 1; nP (sediment) alert no. 8; nP (sediment) alert no. 10; nP (sediment) alert no. 13; nP (sediment) alert no. 22



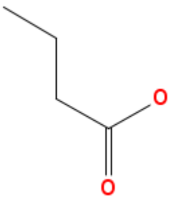
Compound #4

CAS: 79-10-7
Dataset id: 44 (Training set)
SMILES: O=C(O)C=C
Similarity: 0.675

Experimental value: nP
Predicted value: nP

Alerts (found also in the target): nP (sediment) alert no. 1; nP (sediment) alert no. 8; nP (sediment) alert no. 10; nP (sediment) alert no. 13; nP (sediment) alert no. 22

Alerts (not found in the target): nP (sediment) alert no. 11



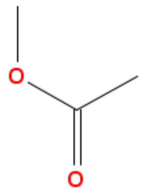
Compound #5

CAS: 107-92-6
Dataset id: 108 (Training set)
SMILES: O=C(O)CCC
Similarity: 0.672

Experimental value: nP
Predicted value: nP

Alerts (found also in the target): nP (sediment) alert no. 1; nP (sediment) alert no. 8; nP (sediment) alert no. 10; nP (sediment) alert no. 13; nP (sediment) alert no. 22

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



Compound #6

CAS: 79-20-9
Dataset id: 46 (Training set)
SMILES: O=C(OC)C
Similarity: 0.664

Experimental value: nP
Predicted value: nP

Alerts (found also in the target): nP (sediment) alert no. 1; nP (sediment) alert no. 8; nP (sediment) alert no. 10

Alerts (not found in the target): nP (sediment) alert no. 14

3.2 Applicability Domain:
Measured Applicability Domain Scores

Global AD Index
AD index = 0.707
Explanation: the predicted compound could be out of the Applicability Domain of the model.

Similar molecules with known experimental value
Similarity index = 0.749
Explanation: only moderately similar compounds with known experimental value in the training set have been found.

Accuracy of prediction for similar molecules
Accuracy index = 0.668
Explanation: accuracy of prediction for similar molecules found in the training set is not optimal.

Concordance for similar molecules
Concordance index = 0.668
Explanation: some similar molecules found in the training set have experimental values that disagree with the predicted value.

Concordance of prediction with found structural alerts
Structural alerts concordance = 1
Explanation: all found alerts are related to experimental values in agreement with the prediction.

Atom Centered Fragments similarity check
ACF index = 1
Explanation: all atom centered fragment of the compound have been found in the compounds of the training set.

Symbols explanation:

The feature has a good assessment, model is reliable regarding this aspect.

The feature has a non optimal assessment, this aspect should be reviewed by an expert.

The feature has a bad assessment, model is not reliable regarding this aspect.

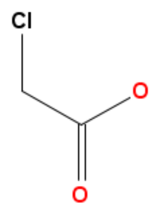
4.1 Reasoning:
Relevant Chemical Fragments and Moieties

(Molecule 0) Reasoning on fragments/structural alerts - 1 of 5:

Fragment found: nP (sediment) alert no. 1

Fragment related to nP compounds (sediment), defined by the SMARTS: O=CC

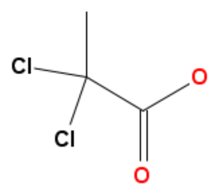
Following, the most similar compounds from the model's dataset having the same fragment.



CAS: 79-11-8
Dataset id: 45 (Training set)
SMILES: C(=O)(O)CCl
Similarity: 0.761

Experimental value: nP
Predicted value: nP

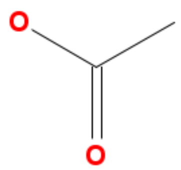
Alerts (found also in the target): nP (sediment) alert no. 1; nP (sediment) alert no. 8; nP (sediment) alert no. 10; nP (sediment) alert no. 13; nP (sediment) alert no. 22



CAS: 75-99-0
Dataset id: 38 (Training set)
SMILES: O=C(O)C(C)(Cl)Cl
Similarity: 0.747

Experimental value: P/vP
Predicted value: nP

Alerts (found also in the target): nP (sediment) alert no. 1; nP (sediment) alert no. 8; nP (sediment) alert no. 10; nP (sediment) alert no. 13; nP (sediment) alert no. 22



CAS: 64-19-7
Dataset id: 17 (Training set)
SMILES: O=C(O)C
Similarity: 0.739

Experimental value: nP
Predicted value: nP

Alerts (found also in the target): nP (sediment) alert no. 1; nP (sediment) alert no. 8; nP (sediment) alert no. 10; nP (sediment) alert no. 13; nP (sediment) alert no. 22

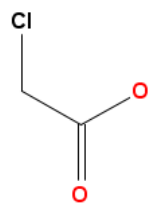
4.1 Reasoning:
Relevant Chemical Fragments and Moieties

(Molecule 0) Reasoning on fragments/structural alerts - 2 of 5:

Fragment found: nP (sediment) alert no. 8

Fragment related to nP compounds (sediment), defined by the SMARTS: C(O)C

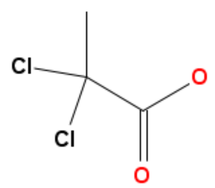
Following, the most similar compounds from the model's dataset having the same fragment.



CAS: 79-11-8
Dataset id: 45 (Training set)
SMILES: C(=O)(O)CCl
Similarity: 0.761

Experimental value: nP
Predicted value: nP

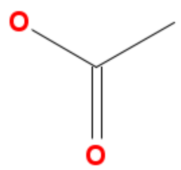
Alerts (found also in the target): nP (sediment) alert no. 1; nP (sediment) alert no. 8; nP (sediment) alert no. 10; nP (sediment) alert no. 13; nP (sediment) alert no. 22



CAS: 75-99-0
Dataset id: 38 (Training set)
SMILES: O=C(O)C(C)(Cl)Cl
Similarity: 0.747

Experimental value: P/vP
Predicted value: nP

Alerts (found also in the target): nP (sediment) alert no. 1; nP (sediment) alert no. 8; nP (sediment) alert no. 10; nP (sediment) alert no. 13; nP (sediment) alert no. 22



CAS: 64-19-7
Dataset id: 17 (Training set)
SMILES: O=C(O)C
Similarity: 0.739

Experimental value: nP
Predicted value: nP

Alerts (found also in the target): nP (sediment) alert no. 1; nP (sediment) alert no. 8; nP (sediment) alert no. 10; nP (sediment) alert no. 13; nP (sediment) alert no. 22

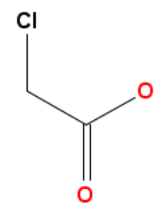
4.1 Reasoning:
Relevant Chemical Fragments and Moieties

(Molecule 0) Reasoning on fragments/structural alerts - 3 of 5:

Fragment found: nP (sediment) alert no. 10

Fragment related to nP compounds (sediment), defined by the SMARTS: O=C

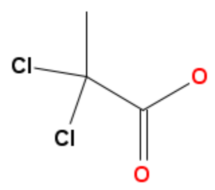
Following, the most similar compounds from the model's dataset having the same fragment.



CAS: 79-11-8
Dataset id: 45 (Training set)
SMILES: C(=O)(O)CCl
Similarity: 0.761

Experimental value: nP
Predicted value: nP

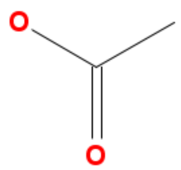
Alerts (found also in the target): nP (sediment) alert no. 1; nP (sediment) alert no. 8; nP (sediment) alert no. 10; nP (sediment) alert no. 13; nP (sediment) alert no. 22



CAS: 75-99-0
Dataset id: 38 (Training set)
SMILES: O=C(O)C(C)(Cl)Cl
Similarity: 0.747

Experimental value: P/vP
Predicted value: nP

Alerts (found also in the target): nP (sediment) alert no. 1; nP (sediment) alert no. 8; nP (sediment) alert no. 10; nP (sediment) alert no. 13; nP (sediment) alert no. 22



CAS: 64-19-7
Dataset id: 17 (Training set)
SMILES: O=C(O)C
Similarity: 0.739

Experimental value: nP
Predicted value: nP

Alerts (found also in the target): nP (sediment) alert no. 1; nP (sediment) alert no. 8; nP (sediment) alert no. 10; nP (sediment) alert no. 13; nP (sediment) alert no. 22

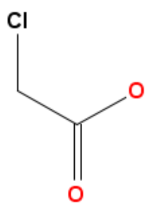
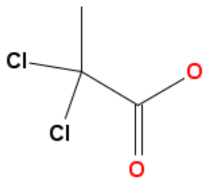
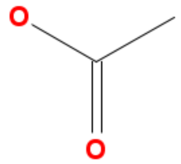
4.1 Reasoning:
Relevant Chemical Fragments and Moieties

(Molecule 0) Reasoning on fragments/structural alerts - 4 of 5:

Fragment found: nP (sediment) alert no. 13

Chemical class related to nP compounds (water), defined by the presence of a single carboxyl acid (aliphatic)

Following, the most similar compounds from the model's dataset having the same fragment.

	CAS: 79-11-8 Dataset id: 45 (Training set) SMILES: C(=O)(O)CCl Similarity: 0.761 Experimental value: nP Predicted value: nP Alerts (found also in the target): nP (sediment) alert no. 1; nP (sediment) alert no. 8; nP (sediment) alert no. 10; nP (sediment) alert no. 13; nP (sediment) alert no. 22
	CAS: 75-99-0 Dataset id: 38 (Training set) SMILES: O=C(O)C(C)(Cl)Cl Similarity: 0.747 Experimental value: P/vP Predicted value: nP Alerts (found also in the target): nP (sediment) alert no. 1; nP (sediment) alert no. 8; nP (sediment) alert no. 10; nP (sediment) alert no. 13; nP (sediment) alert no. 22
	CAS: 64-19-7 Dataset id: 17 (Training set) SMILES: O=C(O)C Similarity: 0.739 Experimental value: nP Predicted value: nP Alerts (found also in the target): nP (sediment) alert no. 1; nP (sediment) alert no. 8; nP (sediment) alert no. 10; nP (sediment) alert no. 13; nP (sediment) alert no. 22

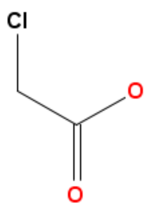
4.1 Reasoning:
Relevant Chemical Fragments and Moieties

(Molecule 0) Reasoning on fragments/structural alerts - 5 of 5:

Fragment found: nP (sediment) alert no. 22

Chemical class related to nP compounds (water), defined by the presence of hydroxyl groups

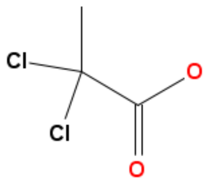
Following, the most similar compounds from the model's dataset having the same fragment.



CAS: 79-11-8
Dataset id: 45 (Training set)
SMILES: C(=O)(O)CCl
Similarity: 0.761

Experimental value: nP
Predicted value: nP

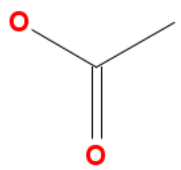
Alerts (found also in the target): nP (sediment) alert no. 1; nP (sediment) alert no. 8; nP (sediment) alert no. 10; nP (sediment) alert no. 13; nP (sediment) alert no. 22



CAS: 75-99-0
Dataset id: 38 (Training set)
SMILES: O=C(O)C(C)(Cl)Cl
Similarity: 0.747

Experimental value: P/vP
Predicted value: nP

Alerts (found also in the target): nP (sediment) alert no. 1; nP (sediment) alert no. 8; nP (sediment) alert no. 10; nP (sediment) alert no. 13; nP (sediment) alert no. 22



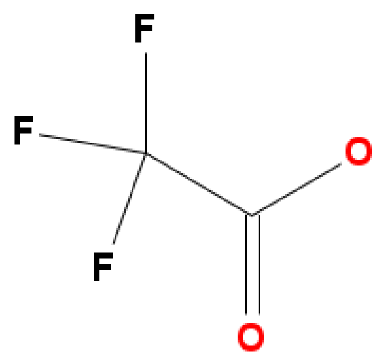
CAS: 64-19-7
Dataset id: 17 (Training set)
SMILES: O=C(O)C
Similarity: 0.739

Experimental value: nP
Predicted value: nP

Alerts (found also in the target): nP (sediment) alert no. 1; nP (sediment) alert no. 8; nP (sediment) alert no. 10; nP (sediment) alert no. 13; nP (sediment) alert no. 22

1. Prediction Summary

Prediction for compound Molecule 0

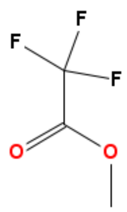


Prediction: Reliability:

Prediction is 0.5, the result appears reliable. Anyhow, you should check it through the evaluation of the information given in the following sections. Anyway some issues could be not optimal:
- only moderately similar compounds with known experimental value in the training set have been found

Compound: Molecule 0
Compound SMILES: O=C(O)C(F)(F)F
Experimental value: -
Predicted LogP: 0.5
Reliability: the predicted compound is into the Applicability Domain of the model
Remarks:
none

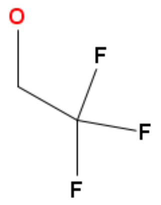
3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



Compound #1

CAS: 431-47-0
Dataset id: 1602 (Training set)
SMILES: O=C(OC)C(F)(F)F
Similarity: 0.895

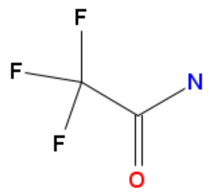
Experimental value: 0.6
Predicted value: 0.789



Compound #2

CAS: 75-89-8
Dataset id: 327 (Training set)
SMILES: FC(F)(F)CO
Similarity: 0.872

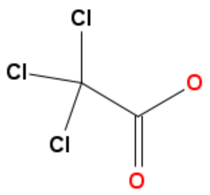
Experimental value: 0.41
Predicted value: 0.275



Compound #3

CAS: 354-38-1
Dataset id: 1536 (Training set)
SMILES: O=C(N)C(F)(F)F
Similarity: 0.853

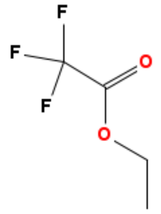
Experimental value: 0.12
Predicted value: -0.746



Compound #4

CAS: 76-03-9
Dataset id: 331 (Training set)
SMILES: O=C(O)C(Cl)(Cl)Cl
Similarity: 0.844

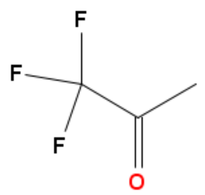
Experimental value: 1.33
Predicted value: 1.442



Compound #5

CAS: 383-63-1
Dataset id: 1573 (Training set)
SMILES: O=C(OCC)C(F)(F)F
Similarity: 0.84

Experimental value: 1.18
Predicted value: 1.28



Compound #6

CAS: 421-50-1
Dataset id: 1597 (Training set)
SMILES: O=C(C)C(F)(F)F
Similarity: 0.836

Experimental value: 0.2
Predicted value: 0.181

3.2 Applicability Domain:
Measured Applicability Domain Scores

✓	**Global AD Index** AD index = 1 Explanation: the predicted compound is into the Applicability Domain of the model.
⚠	**Similar molecules with known experimental value** Similarity index = 0.883 Explanation: only moderately similar compounds with known experimental value in the training set have been found.
✓	**Accuracy of prediction for similar molecules** Accuracy index = 0.162 Explanation: accuracy of prediction for similar molecules found in the training set is good.
✓	**Concordance for similar molecules** Concordance index = 0.095 Explanation: similar molecules found in the training set have experimental values that agree with the predicted value.
✓	**Maximum error of prediction among similar molecules** Max error index = 0.189 Explanation: the maximum error in prediction of similar molecules found in the training set has a low value, considering the experimental variability.

Symbols explanation:

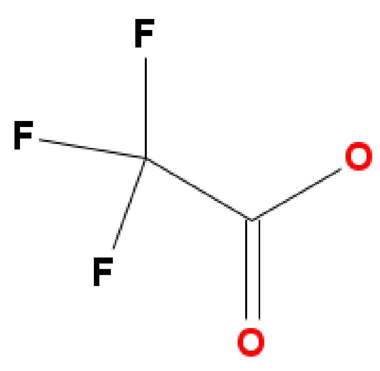
✓ The feature has a good assessment, model is reliable regarding this aspect.

⚠ The feature has a non optimal assessment, this aspect should be reviewed by an expert.

✗ The feature has a bad assessment, model is not reliable regarding this aspect.

1. Prediction Summary

Prediction for compound Molecule 0



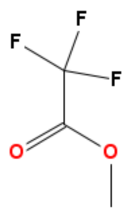
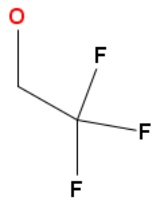
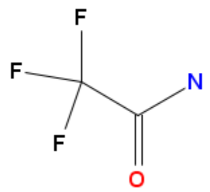
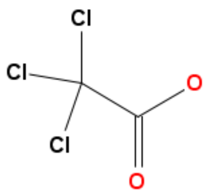
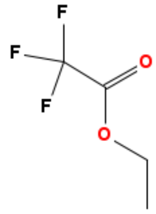
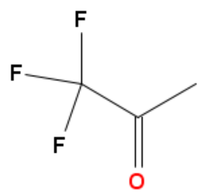
Prediction:

Reliability:

Prediction is 0.37, the result appears reliable. Anyhow, you should check it through the evaluation of the information given in the following sections. Anyway some issues could be not optimal:
- only moderately similar compounds with known experimental value in the training set have been found

Compound: Molecule 0
Compound SMILES: O=C(O)C(F)(F)F
Experimental value: -
Predicted LogP: 0.37
Reliability: the predicted compound is into the Applicability Domain of the model
Remarks:
none

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values

	Compound #1 CAS: 431-47-0 Dataset id: 1602 (Test set) SMILES: O=C(OC)C(F)(F)F Similarity: 0.895 Experimental value: 0.6 Predicted value: 0.795
	Compound #2 CAS: 75-89-8 Dataset id: 327 (Test set) SMILES: FC(F)(F)CO Similarity: 0.872 Experimental value: 0.41 Predicted value: 0.58
	Compound #3 CAS: 354-38-1 Dataset id: 1536 (Test set) SMILES: O=C(N)C(F)(F)F Similarity: 0.853 Experimental value: 0.12 Predicted value: -0.04
	Compound #4 CAS: 76-03-9 Dataset id: 331 (Test set) SMILES: O=C(O)C(Cl)(Cl)Cl Similarity: 0.844 Experimental value: 1.33 Predicted value: 0.996
	Compound #5 CAS: 383-63-1 Dataset id: 1573 (Test set) SMILES: O=C(OCC)C(F)(F)F Similarity: 0.84 Experimental value: 1.18 Predicted value: 1.188
	Compound #6 CAS: 421-50-1 Dataset id: 1597 (Test set) SMILES: O=C(C)C(F)(F)F Similarity: 0.836 Experimental value: 0.2 Predicted value: 0.864

3.2 Applicability Domain:
Measured Applicability Domain Scores

Global AD Index AD index = 1 Explanation: the predicted compound is into the Applicability Domain of the model.
Similar molecules with known experimental value Similarity index = 0.883 Explanation: only moderately similar compounds with known experimental value in the training set have been found.
Accuracy of prediction for similar molecules Accuracy index = 0.183 Explanation: accuracy of prediction for similar molecules found in the training set is good.
Concordance for similar molecules Concordance index = 0.139 Explanation: similar molecules found in the training set have experimental values that agree with the predicted value.
Maximum error of prediction among similar molecules Max error index = 0.195 Explanation: the maximum error in prediction of similar molecules found in the training set has a low value, considering the experimental variability.

Symbols explanation:

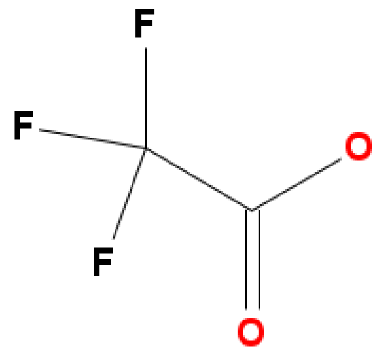
The feature has a good assessment, model is reliable regarding this aspect.

The feature has a non optimal assessment, this aspect should be reviewed by an expert.

The feature has a bad assessment, model is not reliable regarding this aspect.

1. Prediction Summary

Prediction for compound Molecule 0

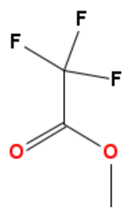


Prediction: Reliability:

Prediction is 0.86, but the result shows some critical aspects, which require to be checked:
- only moderately similar compounds with known experimental value in the training set have been found
- the maximum error in prediction of similar molecules found in the training set has a moderate value, considering the experimental variability

Compound: Molecule 0
Compound SMILES: O=C(O)C(F)(F)F
Experimental value: -
Predicted LogP: 0.86
Reliability: the predicted compound could be out of the Applicability Domain of the model
Remarks:
none

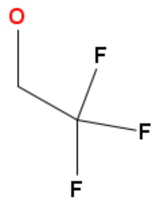
3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



Compound #1

CAS: 431-47-0
Dataset id: 1602 (Test set)
SMILES: O=C(OC)C(F)(F)F
Similarity: 0.895

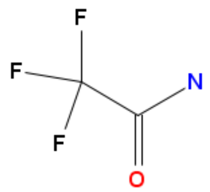
Experimental value: 0.6
Predicted value: 1.109



Compound #2

CAS: 75-89-8
Dataset id: 327 (Test set)
SMILES: FC(F)(F)CO
Similarity: 0.872

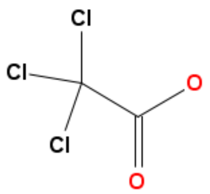
Experimental value: 0.41
Predicted value: 0.649



Compound #3

CAS: 354-38-1
Dataset id: 1536 (Test set)
SMILES: O=C(N)C(F)(F)F
Similarity: 0.853

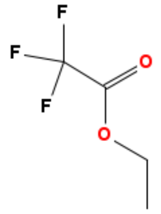
Experimental value: 0.12
Predicted value: 0.256



Compound #4

CAS: 76-03-9
Dataset id: 331 (Test set)
SMILES: O=C(O)C(Cl)(Cl)Cl
Similarity: 0.844

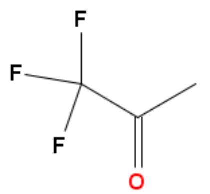
Experimental value: 1.33
Predicted value: 1.448



Compound #5

CAS: 383-63-1
Dataset id: 1573 (Test set)
SMILES: O=C(OCC)C(F)(F)F
Similarity: 0.84

Experimental value: 1.18
Predicted value: 1.458



Compound #6

CAS: 421-50-1
Dataset id: 1597 (Test set)
SMILES: O=C(C)C(F)(F)F
Similarity: 0.836

Experimental value: 0.2
Predicted value: 0.844

3.2 Applicability Domain:
Measured Applicability Domain Scores

Global AD Index
AD index = 0.85
Explanation: the predicted compound could be out of the Applicability Domain of the model.

Similar molecules with known experimental value
Similarity index = 0.883
Explanation: only moderately similar compounds with known experimental value in the training set have been found.

Accuracy of prediction for similar molecules
Accuracy index = 0.374
Explanation: accuracy of prediction for similar molecules found in the training set is good.

Concordance for similar molecules
Concordance index = 0.353
Explanation: similar molecules found in the training set have experimental values that agree with the predicted value.

Maximum error of prediction among similar molecules
Max error index = 0.509
Explanation: the maximum error in prediction of similar molecules found in the training set has a moderate value, considering the experimental variability.

Symbols explanation:

The feature has a good assessment, model is reliable regarding this aspect.

The feature has a non optimal assessment, this aspect should be reviewed by an expert.

The feature has a bad assessment, model is not reliable regarding this aspect.

References and Documentation

You can find complete details on each model and on how to read results in the proper model's guide, available on-line at www.vega-qsar.eu or directly in the VegaNIC application.

Mutagenicity (Ames test) CONSENSUS model (version 1.0.1)

Mutagenicity (Ames test) Consensus model, based on the predictions of the available VEGA mutagenicity models (Caesar, SarPy, ISS and KNN).

Mutagenicity (Ames test) model (CAESAR) (version 2.1.13)

QSAR classification model for Mutagenicity based on a Support Vector Machine combined by a set of ToxTree rules developed by Benigni/Bossa. The model extends the original CAESAR Mutagenicity model 1.0 developed by Politecnico di Milano, Italy. Reference to the original model are found on the CAESAR Project website: http://www.caesar-project.eu/ .

Mutagenicity (Ames test) model (SarPy/IRFMN) (version 1.0.7)

QSAR classification model for Mutagenicity based on a set of rules built with SarPy software. Developed by Istituto Mario Negri, Italy; SarPy software developed by Politecnico di Milano, Italy. Model developed inside the VEGA platform.

Mutagenicity (Ames test) model (ISS) (version 1.0.2)

Classification model for Mutagenicity (Ames test) based on Benigni-Bossa (Istituto Superiore di Sanità) rule set as implemented in ToxTree 2.6.

References and Documentation

Mutagenicity (Ames test) model (KNN/Read-Across) (version 1.0.0)

KNN (Read-Across) model for Mutagenicity (Ames test) developed by Istituto di Ricerche Farmacologiche Mario Negri.

Carcinogenicity model (CAESAR) (version 2.1.9)

QSAR classification model for Carcinogenicity based on a Neural Network. Developed by Kemijski inštitut Ljubljana, Slovenija. The model extends the original CAESAR Carcinogenicity model 1.0 (http://www.caesar-project.eu/). Results are given as membership function values of class Positive and Non-Positive, compound is assigned to the class having value >0.5. Furthermore, structural alerts from ToxTree are searched, providing useful additional information.

Carcinogenicity model (ISS) (version 1.0.2)

Classification model for Carcinogenicity based on Benigni-Bossa (Istituto Superiore di Sanità) rule set as implemented in ToxTree 2.6.

Carcinogenicity model (IRFMN/Antares) (version 1.0.0)

QSAR classification model for Carcinogenicity based on a set of rules built with SarPy software extracted from the Antares dataset. Developed by Istituto Mario Negri, Italy; SarPy software developed by Politecnico di Milano, Italy. Model developed inside the VEGA platform.

VEGA

References and Documentation

Carcinogenicity model (IRFMN/ISSCAN-CGX) (version 1.0.0)

QSAR classification model for Carcinogenicity based on a set of rules built with SarPy software extracted from the ISSCAN-CGX dataset. Developed by Istituto Mario Negri, Italy; SarPy software developed by Politecnico di Milano, Italy. Model developed inside the VEGA platform.

Developmental Toxicity model (CAESAR) (version 2.1.7)

QSAR classification model for Developmental Toxicity based on a Random Forest classification. The model extends the original CAESAR DevTox model 1.0 developed by Istituto Mario Negri, Italy. Reference to the original model are found on the CAESAR Project website: http://www.caesar-project.eu/ .

Developmental/Reproductive Toxicity library (PG) (version 1.0.0)

The model implements a virtual library of toxicant compounds as described in the study from Procter and Gamble: Shengde Wu, Joan Fisher, Jorge M. Naciff, Michael C, Laufersweiler, Cathy Lester, George Daston, and Karen Blackburn "A Framework for Identifying Chemicals with Structural Features Associated with Potential to Act as Developmental or Reproductive Toxicants" Chem. Res. Toxicol., 2013, 26 (12), pp 1840–1861.

Estrogen Receptor Relative Binding Affinity model (IRFMN) (version 1.0.1)

Estrogen Receptor Relative Binding Affinity (RBA) classification model for endocrine disruptor screening based on the model published in A. Roncaglioni, N. Piclin, M. Pintore, E. Benfenati, "Binary classification models for endocrine disrupter effects mediated through the estrogen receptor", SAR and QSAR in Environmental Research (2008), 19, 7-8.

References and Documentation

Estrogen Receptor-mediated effect (IRFMN/CERAPP) (version 1.0.0)

Estrogen Receptor mediated effect classification model for endocrine disruptor screening, based on the the dataset from the CERAPP project (U.S. EPA).

Skin Sensitization model (CAESAR) (version 2.1.6)

QSAR classification model for Skin sensitization based on a Adaptive Fuzzy Partion. The model extends the original CAESAR Skin model 1.0. The original model was developed inside the CAESAR Project (http://www.caesar-project.eu/).

Fish Acute (LC50) Toxicity classification (SarPy/IRFMN) (version 1.0.2)

QSAR classification model for fish acute (LC50) toxicity based on fragments built by SarPy software. Developed by Politecnico di Milano, Italy and Istituto di Ricerche Farmacologiche Mario Negri, Italy.

Fish Acute (LC50) Toxicity model (KNN/Read-Across) (version 1.0.0)

KNN (Read-Across) model for fish acute (LC50) toxicity developed by Istituto di Ricerche Farmacologiche Mario Negri.

References and Documentation

Fish Acute (LC50) Toxicity model (NIC) (version 1.0.0)

QSAR quantitative model for fish acute toxicity based on a Neural Network. Developed by Kemijski inštitut Ljubljana, Slovenija.

Fathead Minnow LC50 96h (EPA) (version 1.0.7)

QSAR model for Fathead Minnow LC50 (96h), based on multiple linear regression. The model extends the original model implemented in the T.E.S.T. software. The original model was developed by US EPA inside the T.E.S.T. software and can be freely accessd at http://www.epa.gov/nrmrl/std/cppb/qsar/.

Daphnia Magna LC50 48h (EPA) (version 1.0.7)

QSAR model for Daphnia Magna LC50 (48h), based on multiple linear regression. The model extends the original model implemented in the T.E.S.T. software. The original model was developed by US EPA inside the T.E.S.T. software and can be freely accessd at http://www.epa.gov/nrmrl/std/cppb/qsar/.

Daphnia Magna LC50 48h (DEMETRA) (version 1.0.4)

Acute toxicity for Water Flea (Daphnia Magna) for pesticides: LC50 48-hours exposure. Built as a Hybrid Model upon two ANNs and a single PLS. Based on the model built for DEMETRA project (http://www.demetra-tox.net).

References and Documentation

Bee acute toxicity model (KNN/IRFMN) (version 1.0.0)

KNN model for bee contact and oral acute toxicity developed by Istituto di Ricerche Farmacologiche Mario Negri.

BCF model (CAESAR) (version 2.1.14)

QSAR model for fish BCF, based on a Radial Basis Function neural network. The model extends the original CAESAR BCF model 1.0, full reference to the model: C. Zhao, E. Boriani, A. Chana, A. Roncaglioni, E. Benfenati "A new hybrid system of QSAR models for predicting bioconcentration factors (BCF)", Chemosphere 73 (2008) 1701–1707. The original model was developed inside the CAESAR Project (http://www.caesar-project.eu/).

BCF model (Meylan) (version 1.0.3)

QSAR model for fish BCF, based on Meylan approach, as implemented in EPI Suite. Full reference to this model can be found in the EPI Suite help (http://www.epa.gov/oppt/exposure/pubs/episuite.htm) and in the original paper from Meylan: Meylan W.M., Howard P.H., Boethling R.S. et al. Improved Method for Estimating Bioconcentration / Bioaccumulation Factor from Octanol/Water Partition Coefficient. 1999, Environ. Toxicol. Chem. 18(4): 664-672. Model developed inside the VEGA platform.

BCF model (KNN/Read-Across) (version 1.1.0)

KNN (Read-Across) model for fish BCF.

References and Documentation

Ready Biodegradability model (IRFMN) (version 1.0.9)

QSAR classification model for Ready Biodegradability based on fragments built by SarPy software. Developed by Politecnico di Milano, Italy and Istituto di Ricerche Farmacologiche Mario Negri, Italy.

Persistence (sediment) model (IRFMN) (version 1.0.0)

Persistence (sediment) model developed by Istituto di Ricerche Farmacologiche Mario Negri.

Persistence (soil) model (IRFMN) (version 1.0.0)

Persistence (soil) model developed by Istituto di Ricerche Farmacologiche Mario Negri.

Persistence (water) model (IRFMN) (version 1.0.0)

Persistence (water) model developed by Istituto di Ricerche Farmacologiche Mario Negri.

References and Documentation

LogP model (Meylan/Kowwin) (version 1.1.4)

LogP prediction based on Meylan work (W.M. Meylan, P.H. Howard, "Atom/fragment contribution method for estimating octanol-water partition coefficients", 1995, J. Pharm. Sci. 84:83-92) and implemented in EPI Suite software as KowWin. Model developed inside the VEGA platform.

LogP model (MLogP) (version 1.0.0)

LogP prediction based on the Moriguchi octanol-water partition coefficient (MLogP), calculated from Moriguchi logP model consisting of a regression equation based on 13 structural parameters (I.Moriguchi, S.Hirono, Q.Liu, I.Nakagome, and Y.Matsushita, Chem.Pharm.Bull. 1992, 40, 127-130; I.Moriguchi, S.Hirono, I.Nakagome, H.Hirano, Chem.Pharm.Bull. 1994, 42, 976-978).

LogP model (ALogP) (version 1.0.0)

LogP prediction based on Ghose-Crippen-Viswanadhan octanol-water partition coefficient (ALogP), calculated from the AlogP model consisting of a regression equation based on the hydrophobicity contribution of 115 atom types (A.K. Ghose and G.M. Crippen, J. Comput. Chem. 1986, 7, 565-577; V.N. Viswanadhan et al., J. Comput. Chem. 1993, 14, 1019-1026; A.K. Ghose, V.N. Viswanadhan, J.J. Wendoloski, J.Phys.Chem. A 1998, 102, 3762-3772).

Annex 4 EUSES Summary 2025 and 2100 Plateau

Printed on	15-12-2017 16:12:35
Study	TFA 2025, low EC50
Substance	Trifluoroacetic acid
Defaults	Standard Euses 2.1
Assessment types	1A, 1B, 2, 3A, 3B
Base set complete	No
Explanation status column	O = Output; D = Default; S = Set; I = Imported

Name	Value	Units	Status
IDENTIFICATION OF THE SUBSTANCE			
General name	Trifluoroacetic acid		S
CAS-No	76-05-1		S
EC-notification no.	200-929-3		S
EINECS no.	200-929-3		S
Molecular weight	114.02	[g.mol-1]	S

Printed on	15-12-2017 16:12:35
Study	Trifluoroacetic acid
Substance	TFA 2025, low EC50
Defaults	Standard Euses 2.1
Assessment types	1A, 1B, 2, 3A, 3B
Base set complete	No

Name	Value	Units	Status
PHYSICO-CHEMICAL PROPERTIES			
Melting point	-15.2	[oC]	S
Boiling point	71.78	[oC]	S
Vapour pressure at test temperature	1.58E+04	[Pa]	S
Vapour pressure at 25 [oC]	1.58E+04	[Pa]	O
Water solubility at test temperature	1E+05	[mg.l-1]	S
Water solubility at 25 [oC]	1E+05	[mg.l-1]	O
Octanol-water partition coefficient	-0.2	[log10]	S
Henry's law constant at 25 [oC]	7.13E-03	[Pa.m3.mol-1]	S

Printed on	15-12-2017 16:12:35
Study	Trifluoroacetic acid
Substance	TFA 2025, low EC50
Defaults	Standard Euses 2.1
Assessment types	1A, 1B, 2, 3A, 3B
Base set complete	No

Name	Value	Units	Status
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
Tonnage of substance in Europe	2E+04	[tonnes.yr-1]	O
Regional production volume of substance	2E+04	[tonnes.yr-1]	O
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
[1 "CHEMICAL PRODUCTION", IC=3/UC=29]			
Industry category	3 Chemical industry: chemicals used in synthesis		S
Use category	29 Heat transferring agents		S
Fraction of tonnage for application	100	[%]	O
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
[PRODUCTION]			
Use specific emission scenario	No		D
Emission tables	A1.1 (general table), B1.6 (general table)		S
Emission scenario	no special scenario selected/available		S
Main category production	Ib Intermed. stored on-site/continuous prod.		S
Fraction of tonnage released to air	1	[-]	S
Fraction of tonnage released to wastewater	0	[-]	S
Fraction of tonnage released to surface water	0	[-]	S
Fraction of tonnage released to industrial soil	0	[-]	S
Fraction of tonnage released to agricultural soil	0	[-]	S
Fraction of the main local source	0.1	[-]	S
Number of emission days per year	240	[-]	S
Local emission to air during episode	7.407E+03	[kg.d-1]	S
Local emission to wastewater during episode	0.152	[kg.d-1]	O
Intermittent release	Yes		S
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
[2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29]			
Industry category	5 Personal / domestic use		S
Use category	29 Heat transferring agents		S
Fraction of tonnage for application	65	[%]	S
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
[PRIVATE USE]			
Use specific emission scenario	No		D
Emission tables	A4.1 (specific uses), B4.1 (general table)		S
Emission scenario	no special scenario selected/available		S
Fraction of tonnage released to air	0.95	[-]	S
Fraction of tonnage released to wastewater	5E-03	[-]	S
Fraction of tonnage released to surface water	0.015	[-]	S
Fraction of tonnage released to industrial soil	0.015	[-]	S
Fraction of tonnage released to agricultural soil	0.015	[-]	S
Fraction of the main local source	2E-03	[-]	O
Number of emission days per year	365	[-]	O
Local emission to air during episode	1	[kg.d-1]	S
Local emission to wastewater during episode	0.164	[kg.d-1]	O
Intermittent release	No		D
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
[3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29]			
Industry category	6 Public domain		S
Use category	29 Heat transferring agents		S
Fraction of tonnage for application	0.35	[-]	S

Name	Value	Units	Status
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
[INDUSTRIAL USE]			
Use specific emission scenario	No		D
Emission tables	A3.5 (specific uses), B3.3 (specific uses)		S
Emission scenario	no special scenario selected/available		S
Fraction of tonnage released to air	0.095	[-]	S
Fraction of tonnage released to wastewater	5E-03	[-]	S
Fraction of tonnage released to surface water	0.015	[-]	S
Fraction of tonnage released to industrial soil	0.015	[-]	S
Fraction of tonnage released to agricultural soil	0.015	[-]	S
Fraction of the main local source	2E-03	[-]	O
Number of emission days per year	50	[-]	O
Local emission to air during episode	10	[kg.d-1]	S
Local emission to wastewater during episode	0.642	[kg.d-1]	O
Intermittent release	No		D
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
TOTAL REGIONAL EMISSIONS TO COMPARTMENTS			
Total regional emission to air	2.3825E+04	[kg.d-1]	S
Total regional emission to wastewater	125	[kg.d-1]	S
Total regional emission to surface water	376	[kg.d-1]	S
Total regional emission to industrial soil	376	[kg.d-1]	S
Total regional emission to agricultural soil	376	[kg.d-1]	S
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
TOTAL CONTINENTAL EMISSIONS TO COMPARTMENTS			
Total continental emission to air	7.1475E+04	[kg.d-1]	S
Total continental emission to wastewater	376	[kg.d-1]	S
Total continental emission to surface water	1.129E+03	[kg.d-1]	S
Total continental emission to industrial soil	1.129E+03	[kg.d-1]	S
Total continental emission to agricultural soil	1.129E+03	[kg.d-1]	S
ENVIRONMENT-EXPOSURE			
PARTITION COEFFICIENTS			
Organic carbon-water partition coefficient	1	[l.kg-1]	S
ENVIRONMENT-EXPOSURE			
DEGRADATION AND TRANSFORMATION			
Characterization of biodegradability	Not biodegradable		S
Degradation calculation method in STP	First order, standard OECD/EU tests		D
Rate constant for biodegradation in STP	0	[d-1]	O
Rate constant for biodegradation in surface water	0	[d-1] (12[oC])	O
Rate constant for biodegradation in bulk soil	6.93E-07	[d-1] (12[oC])	O
Rate constant for biodegradation in aerated sediment	6.93E-07	[d-1] (12[oC])	O
Rate constant for hydrolysis in surface water	6.93E-07	[d-1] (12[oC])	O
Rate constant for photolysis in surface water	6.93E-07	[d-1]	O
ENVIRONMENT-EXPOSURE			
SEWAGE TREATMENT			
LOCAL STP [1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
OUTPUT			
Fraction of emission directed to air by STP	6.83E-03	[%]	O
Fraction of emission directed to water by STP	100	[%]	O
Fraction of emission directed to sludge by STP	0.0125	[%]	O
Fraction of the emission degraded in STP	0	[%]	O
Concentration in untreated wastewater	76	[ug.l-1]	O
Concentration of chemical (total) in the STP-effluent	0.076	[mg.l-1]	O
Concentration in effluent exceeds solubility	No		O
Concentration in dry sewage sludge	0.0241	[mg.kg-1]	O
PEC for micro-organisms in the STP	0.076	[mg.l-1]	O

Name	Value	Units	Status
ENVIRONMENT-EXPOSURE			
SEWAGE TREATMENT			
LOCAL STP [2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
OUTPUT			
Fraction of emission directed to air by STP	6.83E-03	[%]	O
Fraction of emission directed to water by STP	100	[%]	O
Fraction of emission directed to sludge by STP	0.0125	[%]	O
Fraction of the emission degraded in STP	0	[%]	O
Concentration in untreated wastewater	0.082	[mg.l-1]	O
Concentration of chemical (total) in the STP-effluent	0.082	[mg.l-1]	O
Concentration in effluent exceeds solubility	No		O
Concentration in dry sewage sludge	0.026	[mg.kg-1]	O
PEC for micro-organisms in the STP	0.082	[mg.l-1]	O
ENVIRONMENT-EXPOSURE			
SEWAGE TREATMENT			
LOCAL STP [3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
OUTPUT			
Fraction of emission directed to air by STP	6.83E-03	[%]	O
Fraction of emission directed to water by STP	100	[%]	O
Fraction of emission directed to sludge by STP	0.0125	[%]	O
Fraction of the emission degraded in STP	0	[%]	O
Concentration in untreated wastewater	0.321	[mg.l-1]	O
Concentration of chemical (total) in the STP-effluent	0.321	[mg.l-1]	O
Concentration in effluent exceeds solubility	No		O
Concentration in dry sewage sludge	0.102	[mg.kg-1]	O
PEC for micro-organisms in the STP	0.321	[mg.l-1]	O
ENVIRONMENT-EXPOSURE			
SEWAGE TREATMENT			
REGIONAL STP			
Fraction of emission directed to air	10	[%]	S
Fraction of emission directed to water	90	[%]	S
ENVIRONMENT-EXPOSURE			
SEWAGE TREATMENT			
CONTINENTAL STP			
Fraction of emission directed to air	10	[%]	S
Fraction of emission directed to water	90	[%]	S
Fraction of the emission degraded	0	[%]	S
ENVIRONMENT-EXPOSURE			
DISTRIBUTION			
LOCAL SCALE			
[1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
Concentration in air during emission episode	2.9E-08	[mg.m-3]	S
Annual average concentration in air, 100 m from point source	1.91E-08	[mg.m-3]	O
Concentration in surface water during emission episode (dissolved)	7.6E-03	[mg.l-1]	O
Annual average concentration in surface water (dissolved)	5E-03	[mg.l-1]	O
Local PEC in surface water during emission episode (dissolved)	7.93E-03	[mg.l-1]	O
Annual average local PEC in surface water (dissolved)	5.33E-03	[mg.l-1]	O
Local PEC in fresh-water sediment during emission episode	6.38E-03	[mg.kgwwt-1]	O
Concentration in seawater during emission episode (dissolved)	7.6E-04	[mg.l-1]	O
Annual average concentration in seawater (dissolved)	5E-04	[mg.l-1]	O
Local PEC in seawater during emission episode (dissolved)	9.6E-04	[mg.l-1]	O
Annual average local PEC in seawater (dissolved)	7E-04	[mg.l-1]	O
Local PEC in marine sediment during emission episode	7.72E-04	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 30 days	0.571	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 180 days	0.571	[mg.kgwwt-1]	O
Local PEC in grassland (total) averaged over 180 days	0.571	[mg.kgwwt-1]	O
Local PEC in groundwater under agricultural soil	4.22	[mg.l-1]	O

Name	Value	Units	Status
ENVIRONMENT-EXPOSURE			
DISTRIBUTION			
LOCAL SCALE			
[2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
Concentration in air during emission episode	2.78E-04	[mg.m-3]	O
Annual average concentration in air, 100 m from point source	2.78E-04	[mg.m-3]	O
Concentration in surface water during emission episode (dissolved)	8.2E-03	[mg.l-1]	O
Annual average concentration in surface water (dissolved)	8.2E-03	[mg.l-1]	O
Local PEC in surface water during emission episode (dissolved)	8.53E-03	[mg.l-1]	O
Annual average local PEC in surface water (dissolved)	8.53E-03	[mg.l-1]	O
Local PEC in fresh-water sediment during emission episode	6.86E-03	[mg.kgwwt-1]	O
Concentration in seawater during emission episode (dissolved)	8.2E-04	[mg.l-1]	O
Annual average concentration in seawater (dissolved)	8.2E-04	[mg.l-1]	O
Local PEC in seawater during emission episode (dissolved)	1.02E-03	[mg.l-1]	O
Annual average local PEC in seawater (dissolved)	1.02E-03	[mg.l-1]	O
Local PEC in marine sediment during emission episode	8.2E-04	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 30 days	5.15E-03	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 180 days	5.13E-03	[mg.kgwwt-1]	O
Local PEC in grassland (total) averaged over 180 days	5.12E-03	[mg.kgwwt-1]	O
Local PEC in groundwater under agricultural soil	0.0379	[mg.l-1]	O
ENVIRONMENT-EXPOSURE			
DISTRIBUTION			
LOCAL SCALE			
[3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
Concentration in air during emission episode	2.78E-03	[mg.m-3]	O
Annual average concentration in air, 100 m from point source	3.81E-04	[mg.m-3]	O
Concentration in surface water during emission episode (dissolved)	0.0321	[mg.l-1]	O
Annual average concentration in surface water (dissolved)	4.4E-03	[mg.l-1]	O
Local PEC in surface water during emission episode (dissolved)	0.0324	[mg.l-1]	O
Annual average local PEC in surface water (dissolved)	4.73E-03	[mg.l-1]	O
Local PEC in fresh-water sediment during emission episode	0.0261	[mg.kgwwt-1]	O
Concentration in seawater during emission episode (dissolved)	3.21E-03	[mg.l-1]	O
Annual average concentration in seawater (dissolved)	4.4E-04	[mg.l-1]	O
Local PEC in seawater during emission episode (dissolved)	3.41E-03	[mg.l-1]	O
Annual average local PEC in seawater (dissolved)	6.4E-04	[mg.l-1]	O
Local PEC in marine sediment during emission episode	2.74E-03	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 30 days	5.28E-03	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 180 days	5.22E-03	[mg.kgwwt-1]	O
Local PEC in grassland (total) averaged over 180 days	5.17E-03	[mg.kgwwt-1]	O
Local PEC in groundwater under agricultural soil	0.0386	[mg.l-1]	O
ENVIRONMENT-EXPOSURE			
DISTRIBUTION			
REGIONAL AND CONTINENTAL SCALE			
CONTINENTAL			
Continental PEC in surface water (dissolved)	3.5E-04	[mg.l-1]	O
Continental PEC in seawater (dissolved)	2.72E-04	[mg.l-1]	O
Continental PEC in air (total)	1.04E-03	[mg.m-3]	O
Continental PEC in agricultural soil (total)	1.16E-04	[mg.kgwwt-1]	O
Continental PEC in pore water of agricultural soils	8.51E-04	[mg.l-1]	O
Continental PEC in natural soil (total)	6.48E-05	[mg.kgwwt-1]	O
Continental PEC in industrial soil (total)	3.69E-04	[mg.kgwwt-1]	O
Continental PEC in sediment (total)	2.45E-04	[mg.kgwwt-1]	O
Continental PEC in seawater sediment (total)	1.94E-04	[mg.kgwwt-1]	O

Name	Value	Units	Status
ENVIRONMENT-EXPOSURE			
DISTRIBUTION			
REGIONAL AND CONTINENTAL SCALE			
REGIONAL			
Regional PEC in surface water (dissolved)	3.28E-04	[mg.l-1]	S
Regional PEC in seawater (dissolved)	2E-04	[mg.l-1]	S
Regional PEC in air (total)	4.1E-09	[mg.m-3]	S
Regional PEC in agricultural soil (total)	5E-03	[mg.kgwwt-1]	S
Regional PEC in pore water of agricultural soils	3.28E-04	[mg.l-1]	S
Regional PEC in natural soil (total)	5E-03	[mg.kgwwt-1]	S
Regional PEC in industrial soil (total)	5E-03	[mg.kgwwt-1]	S
Regional PEC in sediment (total)	5E-03	[mg.kgwwt-1]	S
Regional PEC in seawater sediment (total)	5E-03	[mg.kgwwt-1]	S
ENVIRONMENT-EXPOSURE			
BIOCONCENTRATION			
Bioconcentration factor for earthworms	0.848	[l.kgwwt-1]	O
Bioconcentration factor for fish	1.41	[l.kgwwt-1]	O
ENVIRONMENT-EXPOSURE			
SECONDARY POISONING [1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
Concentration in fish for secondary poisoning (freshwater)	3.99E-03	[mg.kgwwt-1]	O
Concentration in fish for secondary poisoning (marine)	6.36E-04	[mg.kgwwt-1]	O
Concentration in fish-eating marine top-predators	3.53E-04	[mg.kgwwt-1]	O
Concentration in earthworms from agricultural soil	1.64	[mg.kg-1]	O
ENVIRONMENT-EXPOSURE			
SECONDARY POISONING [2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
Concentration in fish for secondary poisoning (freshwater)	6.25E-03	[mg.kgwwt-1]	O
Concentration in fish for secondary poisoning (marine)	8.62E-04	[mg.kgwwt-1]	O
Concentration in fish-eating marine top-predators	3.98E-04	[mg.kgwwt-1]	O
Concentration in earthworms from agricultural soil	0.0151	[mg.kg-1]	O
ENVIRONMENT-EXPOSURE			
SECONDARY POISONING [3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
Concentration in fish for secondary poisoning (freshwater)	3.57E-03	[mg.kgwwt-1]	O
Concentration in fish for secondary poisoning (marine)	5.93E-04	[mg.kgwwt-1]	O
Concentration in fish-eating marine top-predators	3.45E-04	[mg.kgwwt-1]	O
Concentration in earthworms from agricultural soil	0.0153	[mg.kg-1]	O

Name	Value	Units	Status
ENVIRONMENT - EFFECTS			
MICRO-ORGANISMS			
Test system	Respiration inhibition, EU Annex V C.11, OECD 209 D		
EC50 for micro-organisms in a STP	832	[mg.l-1]	S
EC10 for micro-organisms in a STP	832	[mg.l-1]	S
NOEC for micro-organisms in a STP	832	[mg.l-1]	S
PNEC for micro-organisms in a STP	8.32	[mg.l-1]	O
Assessment factor applied in extrapolation to PNEC micro	10	[-]	S
ENVIRONMENT - EFFECTS			
FRESH_WATER ORGANISMS			
LC50 for fish	1.2E+03	[mg.l-1]	S
L(E)C50 for Daphnia	1.2E+03	[mg.l-1]	S
EC50 for algae	0.62	[mg.l-1]	S
LC50 for additional taxonomic group	??	[mg.l-1]	D
NOEC for fish	??	[mg.l-1]	D
NOEC for Daphnia	??	[mg.l-1]	D
NOEC for algae	??	[mg.l-1]	D
NOEC for additional taxonomic group	??	[mg.l-1]	D
PNEC for aquatic organisms	6.2E-04	[mg.l-1]	O
PNEC for aquatic organisms, intermittent releases	6.2E-03	[mg.l-1]	O
ENVIRONMENT - EFFECTS			
MARINE ORGANISMS			
LC50 for fish (marine)	??	[mg.l-1]	D
L(E)C50 for crustaceans (marine)	??	[mg.l-1]	D
EC50 for algae (marine)	97	[mg.l-1]	S
LC50 for additional taxonomic group (marine)	??	[mg.l-1]	D
NOEC for fish (marine)	??	[mg.l-1]	D
NOEC for crustaceans (marine)	??	[mg.l-1]	D
NOEC for algae (marine)	??	[mg.l-1]	D
NOEC for additional taxonomic group (marine)	??	[mg.l-1]	D
PNEC for marine organisms	6.2E-05	[mg.l-1]	O
ENVIRONMENT - EFFECTS			
FRESH-WATER SEDIMENT ORGANISMS			
LC50 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
PNEC for fresh-water sediment, normalised to 5% o.c. (regional)	4.99E-04	[mg.kgwwt-1]	O
ENVIRONMENT - EFFECTS			
MARINE SEDIMENT ORGANISMS			
LC50 for marine sediment organism	??	[mg.kgwwt-1]	D
EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D
PNEC for marine sediment, normalised to 5% o.c. (regional)	4.99E-05	[mg.kgwwt-1]	O

Name	Value	Units	Status
ENVIRONMENT - EFFECTS			
TERRESTRIAL ORGANISMS			
LC50 for plants	250	[mg.kgdwt-1]	S
LC50 for earthworms	??	[mg.kgwwt-1]	D
EC50 for microorganisms	??	[mg.kgwwt-1]	D
LC50 for other terrestrial species	??	[mg.kgwwt-1]	D
NOEC for plants	??	[mg.kgwwt-1]	D
NOEC for earthworms	??	[mg.kgwwt-1]	D
NOEC for microorganisms	??	[mg.kgwwt-1]	D
NOEC for additional taxonomic group	??	[mg.kgwwt-1]	D
NOEC for additional taxonomic group	??	[mg.kgwwt-1]	D
PNEC for terrestrial organisms	8.39E-05	[mg.kgwwt-1]	O
Equilibrium partitioning used for PNEC in soil?	Yes		O
ENVIRONMENT - EFFECTS			
BIRDS AND MAMMALS			
Oral NOAEL (repdose)	1E+03	[mg.kg-1.d-1]	S
NOEC via food (repdose)	1E+04	[mg.kg-1]	O
Inhalatory NOAEL (repdose)	1.75E+03	[mg.m-3]	O
Dermal NOAEL (repdose)	1E+03	[mg.kg-1.d-1]	O
Oral NOAEL (fert)	1E+03	[mg.kg-1.d-1]	S
NOEC via food (fert)	1E+04	[mg.kg-1]	O
Inhalatory NOAEL (fert)	1.75E+03	[mg.m-3]	O
Dermal NOAEL (fert)	1E+03	[mg.kg-1.d-1]	O
Oral NOAEL (mattox)	150	[mg.kg-1.d-1]	S
NOEC via food (mattox)	1.5E+03	[mg.kg-1]	O
Inhalatory NOAEL (mattox)	262	[mg.m-3]	O
Dermal NOAEL (mattox)	150	[mg.kg-1.d-1]	O
Oral NOAEL (devtox)	150	[mg.kg-1.d-1]	S
NOEC via food (devtox)	1.5E+03	[mg.kg-1]	O
Inhalatory NOAEL (devtox)	262	[mg.m-3]	O
Dermal NOAEL (devtox)	150	[mg.kg-1.d-1]	O
Duration of (sub-)chronic oral test	28 days		D
NOEC via food for secondary poisoning	1E+04	[mg.kg-1]	O
PNEC for secondary poisoning of birds and mammals	33.3	[mg.kg-1]	O

Name	Value	Units	Status
ENVIRONMENT - RISK CHARACTERIZATION			
LOCAL [1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
RCR for the local fresh-water compartment	1.28	[-]	O
RCR for the local fresh-water compartment, statistical method	??	[-]	O
RCR for the local marine compartment	15.5	[-]	O
RCR for the local marine compartment, statistical method	??	[-]	O
RCR for the local fresh-water sediment compartment	12.8	[-]	O
RCR for the local marine sediment compartment	15.5	[-]	O
RCR for the local soil compartment	6.81E+03	[-]	O
RCR for the local soil compartment, statistical method	??	[-]	O
RCR for the sewage treatment plant	9.14E-03	[-]	O
RCR for fish-eating birds and mammals (fresh-water)	1.2E-04	[-]	O
RCR for fish-eating birds and mammals (marine)	1.91E-05	[-]	O
RCR for top predators (marine)	1.06E-05	[-]	O
RCR for worm-eating birds and mammals	0.0491	[-]	O
ENVIRONMENT - RISK CHARACTERIZATION			
LOCAL [2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
RCR for the local fresh-water compartment	13.8	[-]	O
RCR for the local fresh-water compartment, statistical method	??	[-]	O
RCR for the local marine compartment	16.5	[-]	O
RCR for the local marine compartment, statistical method	??	[-]	O
RCR for the local fresh-water sediment compartment	13.8	[-]	O
RCR for the local marine sediment compartment	16.5	[-]	O
RCR for the local soil compartment	61.4	[-]	O
RCR for the local soil compartment, statistical method	??	[-]	O
RCR for the sewage treatment plant	9.85E-03	[-]	O
RCR for fish-eating birds and mammals (fresh-water)	1.88E-04	[-]	O
RCR for fish-eating birds and mammals (marine)	2.58E-05	[-]	O
RCR for top predators (marine)	1.2E-05	[-]	O
RCR for worm-eating birds and mammals	4.52E-04	[-]	O
ENVIRONMENT - RISK CHARACTERIZATION			
LOCAL [3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
RCR for the local fresh-water compartment	52.3	[-]	O
RCR for the local fresh-water compartment, statistical method	??	[-]	O
RCR for the local marine compartment	55	[-]	O
RCR for the local marine compartment, statistical method	??	[-]	O
RCR for the local fresh-water sediment compartment	52.3	[-]	O
RCR for the local marine sediment compartment	55	[-]	O
RCR for the local soil compartment	63	[-]	O
RCR for the local soil compartment, statistical method	??	[-]	O
RCR for the sewage treatment plant	0.0386	[-]	O
RCR for fish-eating birds and mammals (fresh-water)	1.07E-04	[-]	O
RCR for fish-eating birds and mammals (marine)	1.78E-05	[-]	O
RCR for top predators (marine)	1.03E-05	[-]	O
RCR for worm-eating birds and mammals	4.6E-04	[-]	O
ENVIRONMENT - RISK CHARACTERIZATION			
REGIONAL			
RCR for the regional fresh-water compartment	0.529	[-]	O
RCR for the regional fresh-water compartment, statistical method	??	[-]	O
RCR for the regional marine compartment	3.23	[-]	O
RCR for the regional marine compartment, statistical method	??	[-]	O
RCR for the regional fresh-water sediment compartment	10	[-]	O
RCR for the regional marine sediment compartment	100	[-]	O
RCR for the regional soil compartment	59.6	[-]	O
RCR for the regional soil compartment, statistical method	??	[-]	O

Name	Value	Units	Status
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
Purification factor for surface water	1	[-]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
CONCENTRATIONS IN INTAKE MEDIA [1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
Local concentration in wet fish	7.52E-03	[mg.kg-1]	O
Local concentration in root tissue of plant	3.96	[mg.kg-1]	O
Local concentration in leaves of plant	0.931	[mg.kg-1]	O
Local concentration in grass (wet weight)	0.931	[mg.kg-1]	O
Local concentration in drinking water	4.22	[mg.l-1]	O
Local concentration in meat (wet weight)	2.35E-04	[mg.kg-1]	O
Local concentration in milk (wet weight)	2.35E-03	[mg.kg-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
DOSES IN INTAKE MEDIA [1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
Daily dose through intake of drinking water	0.121	[mg.kg-1.d-1]	O
Daily dose through intake of fish	1.24E-05	[mg.kg-1.d-1]	O
Daily dose through intake of leaf crops	0.016	[mg.kg-1.d-1]	O
Daily dose through intake of root crops	0.0217	[mg.kg-1.d-1]	O
Daily dose through intake of meat	1.01E-06	[mg.kg-1.d-1]	O
Daily dose through intake of milk	1.88E-05	[mg.kg-1.d-1]	O
Daily dose through intake of air	6.62E-09	[mg.kg-1.d-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
FRACTIONS OF TOTAL DOSE [1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
Fraction of total dose through intake of drinking water	0.762	[-]	O
Fraction of total dose through intake of fish	7.81E-05	[-]	O
Fraction of total dose through intake of leaf crops	0.101	[-]	O
Fraction of total dose through intake of root crops	0.137	[-]	O
Fraction of total dose through intake of meat	6.37E-06	[-]	O
Fraction of total dose through intake of milk	1.19E-04	[-]	O
Fraction of total dose through intake of air	4.18E-08	[-]	O
Local total daily intake for humans	0.158	[mg.kg-1.d-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
CONCENTRATIONS IN INTAKE MEDIA [2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
Local concentration in wet fish	0.012	[mg.kg-1]	O
Local concentration in root tissue of plant	0.0356	[mg.kg-1]	O
Local concentration in leaves of plant	0.177	[mg.kg-1]	O
Local concentration in grass (wet weight)	0.177	[mg.kg-1]	O
Local concentration in drinking water	0.0379	[mg.l-1]	O
Local concentration in meat (wet weight)	1.12E-05	[mg.kg-1]	O
Local concentration in milk (wet weight)	1.12E-04	[mg.kg-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
DOSES IN INTAKE MEDIA [2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
Daily dose through intake of drinking water	1.08E-03	[mg.kg-1.d-1]	O
Daily dose through intake of fish	1.98E-05	[mg.kg-1.d-1]	O
Daily dose through intake of leaf crops	3.03E-03	[mg.kg-1.d-1]	O
Daily dose through intake of root crops	1.95E-04	[mg.kg-1.d-1]	O
Daily dose through intake of meat	4.81E-08	[mg.kg-1.d-1]	O
Daily dose through intake of milk	8.96E-07	[mg.kg-1.d-1]	O
Daily dose through intake of air	7.94E-05	[mg.kg-1.d-1]	O

Name	Value	Units	Status
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
FRACTIONS OF TOTAL DOSE [2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
Fraction of total dose through intake of drinking water	0.246	[-]	O
Fraction of total dose through intake of fish	4.49E-03	[-]	O
Fraction of total dose through intake of leaf crops	0.687	[-]	O
Fraction of total dose through intake of root crops	0.0442	[-]	O
Fraction of total dose through intake of meat	1.09E-05	[-]	O
Fraction of total dose through intake of milk	2.03E-04	[-]	O
Fraction of total dose through intake of air	0.018	[-]	O
Local total daily intake for humans	4.41E-03	[mg.kg-1.d-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
CONCENTRATIONS IN INTAKE MEDIA [3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
Local concentration in wet fish	6.68E-03	[mg.kg-1]	O
Local concentration in root tissue of plant	0.0362	[mg.kg-1]	O
Local concentration in leaves of plant	0.239	[mg.kg-1]	O
Local concentration in grass (wet weight)	0.239	[mg.kg-1]	O
Local concentration in drinking water	0.0386	[mg.l-1]	O
Local concentration in meat (wet weight)	1.46E-05	[mg.kg-1]	O
Local concentration in milk (wet weight)	1.46E-04	[mg.kg-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
DOSES IN INTAKE MEDIA [3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
Daily dose through intake of drinking water	1.1E-03	[mg.kg-1.d-1]	O
Daily dose through intake of fish	1.1E-05	[mg.kg-1.d-1]	O
Daily dose through intake of leaf crops	4.1E-03	[mg.kg-1.d-1]	O
Daily dose through intake of root crops	1.98E-04	[mg.kg-1.d-1]	O
Daily dose through intake of meat	6.27E-08	[mg.kg-1.d-1]	O
Daily dose through intake of milk	1.17E-06	[mg.kg-1.d-1]	O
Daily dose through intake of air	1.09E-04	[mg.kg-1.d-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
FRACTIONS OF TOTAL DOSE [3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
Fraction of total dose through intake of drinking water	0.2	[-]	O
Fraction of total dose through intake of fish	1.99E-03	[-]	O
Fraction of total dose through intake of leaf crops	0.743	[-]	O
Fraction of total dose through intake of root crops	0.0359	[-]	O
Fraction of total dose through intake of meat	1.13E-05	[-]	O
Fraction of total dose through intake of milk	2.11E-04	[-]	O
Fraction of total dose through intake of air	0.0197	[-]	O
Local total daily intake for humans	5.52E-03	[mg.kg-1.d-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
REGIONAL SCALE			
CONCENTRATIONS IN INTAKE MEDIA			
Regional concentration in wet fish	4.63E-04	[mg.kg-1]	O
Regional concentration in root tissue of plant	3.08E-04	[mg.kg-1]	O
Regional concentration in leaves of plant	7.48E-05	[mg.kg-1]	O
Regional concentration in grass (wet weight)	7.48E-05	[mg.kg-1]	O
Regional concentration in drinking water	1.23E-04	[mg.l-1]	S
Regional concentration in meat (wet weight)	1.12E-08	[mg.kg-1]	O
Regional concentration in milk (wet weight)	1.12E-07	[mg.kg-1]	O

Printed on	15-12-2017 16:12:35
Study	Trifluoroacetic acid
Substance	TFA 2025, low EC50
Defaults	Standard Euses 2.1
Assessment types	1A, 1B, 2, 3A, 3B
Base set complete	No

Name	Value	Units	Status
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
REGIONAL SCALE			
DOSES IN INTAKE MEDIA			
Daily dose through intake of drinking water	3.51E-06	[mg.kg-1.d-1]	O
Daily dose through intake of fish	7.61E-07	[mg.kg-1.d-1]	O
Daily dose through intake of leaf crops	1.28E-06	[mg.kg-1.d-1]	O
Daily dose through intake of root crops	1.69E-06	[mg.kg-1.d-1]	O
Daily dose through intake of meat	4.83E-11	[mg.kg-1.d-1]	O
Daily dose through intake of milk	9.01E-10	[mg.kg-1.d-1]	O
Daily dose through intake of air	1.17E-09	[mg.kg-1.d-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
REGIONAL SCALE			
FRACTIONS OF TOTAL DOSE			
Fraction of total dose through intake of drinking water	0.485	[-]	O
Fraction of total dose through intake of fish	0.105	[-]	O
Fraction of total dose through intake of leaf crops	0.177	[-]	O
Fraction of total dose through intake of root crops	0.233	[-]	O
Fraction of total dose through intake of meat	6.67E-06	[-]	O
Fraction of total dose through intake of milk	1.24E-04	[-]	O
Fraction of total dose through intake of air	1.62E-04	[-]	O
Regional total daily intake for humans	7.25E-06	[mg.kg-1.d-1]	O

Name	Value	Units	Status
HUMAN HEALTH - RISK CHARACTERIZATION			
CURRENT CLASSIFICATION			
Corrosive (C, R34 or R35)	Yes		S
Irritating to skin (Xi, R38)	No		D
Irritating to eyes (Xi, R36)	No		D
Risk of serious damage to eyes (Xi, R41)	No		D
Irritating to respiratory system (Xi, R37)	No		D
May cause sensitisation by inhalation (Xn, R42)	No		D
May cause sensitisation by skin contact (Xi, R43)	No		D
May cause cancer (T, R45)	No		D
May cause cancer by inhalation (T, R49)	No		D
Possible risk of irreversible effects (Xn, R40)	No		D
HUMAN HEALTH - RISK CHARACTERIZATION			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL [1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
MOS, local, inhalatory (repdose)	7.55E+10	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (repdose)	7.55E+10	[-]	O
MOS, local, total exposure (repdose)	6.32E+03	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (repdose)	6.32E+03	[-]	O
MOS, local, inhalatory (fert)	7.55E+10	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (fert)	7.55E+10	[-]	O
MOS, local, total exposure (fert)	6.32E+03	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (fert)	6.32E+03	[-]	O
MOS, local, inhalatory (mattox)	1.13E+10	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (mattox)	1.13E+10	[-]	O
MOS, local, total exposure (mattox)	947	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (mattox)	947	[-]	O
MOS, local, inhalatory (devtox)	1.13E+10	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (devtox)	1.13E+10	[-]	O
MOS, local, total exposure (devtox)	947	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (devtox)	947	[-]	O
HUMAN HEALTH - RISK CHARACTERIZATION			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL [2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
MOS, local, inhalatory (repdose)	6.29E+06	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (repdose)	6.29E+06	[-]	O
MOS, local, total exposure (repdose)	2.27E+05	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (repdose)	2.27E+05	[-]	O
MOS, local, inhalatory (fert)	6.29E+06	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (fert)	6.29E+06	[-]	O
MOS, local, total exposure (fert)	2.27E+05	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (fert)	2.27E+05	[-]	O
MOS, local, inhalatory (mattox)	9.44E+05	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (mattox)	9.44E+05	[-]	O
MOS, local, total exposure (mattox)	3.4E+04	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (mattox)	3.4E+04	[-]	O
MOS, local, inhalatory (devtox)	9.44E+05	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (devtox)	9.44E+05	[-]	O
MOS, local, total exposure (devtox)	3.4E+04	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (devtox)	3.4E+04	[-]	O

Name	Value	Units	Status
HUMAN HEALTH - RISK CHARACTERIZATION			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL [3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
MOS, local, inhalatory (repdose)	4.6E+06	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (repdose)	4.6E+06	[-]	O
MOS, local, total exposure (repdose)	1.81E+05	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (repdose)	1.81E+05	[-]	O
MOS, local, inhalatory (fert)	4.6E+06	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (fert)	4.6E+06	[-]	O
MOS, local, total exposure (fert)	1.81E+05	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (fert)	1.81E+05	[-]	O
MOS, local, inhalatory (mattox)	6.89E+05	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (mattox)	6.89E+05	[-]	O
MOS, local, total exposure (mattox)	2.72E+04	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (mattox)	2.72E+04	[-]	O
MOS, local, inhalatory (devtox)	6.89E+05	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (devtox)	6.89E+05	[-]	O
MOS, local, total exposure (devtox)	2.72E+04	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (devtox)	2.72E+04	[-]	O
HUMAN HEALTH - RISK CHARACTERIZATION			
HUMANS EXPOSED VIA THE ENVIRONMENT			
REGIONAL			
MOS, regional, inhalatory (repdose)	4.27E+11	[-]	O
Ratio MOS/Ref-MOS, regional, inhalatory (repdose)	4.27E+11	[-]	O
MOS, regional, total exposure (repdose)	1.38E+08	[-]	O
Ratio MOS/Ref-MOS, regional, total exposure (repdose)	1.38E+08	[-]	O
MOS, regional, inhalatory (fert)	4.27E+11	[-]	O
Ratio MOS/Ref-MOS, regional, inhalatory (fert)	4.27E+11	[-]	O
MOS, regional, total exposure (fert)	1.38E+08	[-]	O
Ratio MOS/Ref-MOS, regional, total exposure (fert)	1.38E+08	[-]	O
MOS, regional, inhalatory (mattox)	6.4E+10	[-]	O
Ratio MOS/Ref-MOS, regional, inhalatory (mattox)	6.4E+10	[-]	O
MOS, regional, total exposure (mattox)	2.07E+07	[-]	O
Ratio MOS/Ref-MOS, regional, total exposure (mattox)	2.07E+07	[-]	O
MOS, regional, inhalatory (devtox)	6.4E+10	[-]	O
Ratio MOS/Ref-MOS, regional, inhalatory (devtox)	6.4E+10	[-]	O
MOS, regional, total exposure (devtox)	2.07E+07	[-]	O
Ratio MOS/Ref-MOS, regional, total exposure (devtox)	2.07E+07	[-]	O

EUSES 2 Summary report	Single substance
Printed on	15-12-2017 16:53:50
Study	TFA 2025 mid EC50
Substance	Trifluoroacetic acid
Defaults	Standard Euses 2.1
Assessment types	1A, 1B, 2, 3A, 3B
Base set complete	No
Explanation status column	O = Output; D = Default; S = Set; I = Imported

Name	Value	Units	Status
IDENTIFICATION OF THE SUBSTANCE			
General name	Trifluoroacetic acid		S
CAS-No	76-05-1		S
EC-notification no.	200-929-3		S
EINECS no.	200-929-3		S
Molecular weight	114.02	[g.mol-1]	S

Printed on	15-12-2017 16:53:50
Study	Trifluoroacetic acid
Substance	TFA 2025 mid EC50
Defaults	Standard Euses 2.1
Assessment types	1A, 1B, 2, 3A, 3B
Base set complete	No

Name	Value	Units	Status
PHYSICO-CHEMICAL PROPERTIES			
Melting point	-15.2	[oC]	S
Boiling point	71.78	[oC]	S
Vapour pressure at test temperature	1.58E+04	[Pa]	S
Vapour pressure at 25 [oC]	1.58E+04	[Pa]	O
Water solubility at test temperature	1E+05	[mg.l-1]	S
Water solubility at 25 [oC]	1E+05	[mg.l-1]	O
Octanol-water partition coefficient	-0.2	[log10]	S
Henry's law constant at 25 [oC]	7.13E-03	[Pa.m3.mol-1]	S

Printed on	15-12-2017 16:53:50
Study	Trifluoroacetic acid
Substance	TFA 2025 mid EC50
Defaults	Standard Euses 2.1
Assessment types	1A, 1B, 2, 3A, 3B
Base set complete	No

Name	Value	Units	Status
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
Tonnage of substance in Europe	2E+04	[tonnes.yr-1]	O
Regional production volume of substance	2E+04	[tonnes.yr-1]	O
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
[1 "CHEMICAL PRODUCTION", IC=3/UC=29]			
Industry category	3 Chemical industry: chemicals used in synthesis		S
Use category	29 Heat transferring agents		S
Fraction of tonnage for application	100	[%]	O
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
[PRODUCTION]			
Use specific emission scenario	No		D
Emission tables	A1.1 (general table), B1.6 (general table)		S
Emission scenario	no special scenario selected/available		S
Main category production	Ib Intermed. stored on-site/continuous prod.		S
Fraction of tonnage released to air	1	[-]	S
Fraction of tonnage released to wastewater	0	[-]	S
Fraction of tonnage released to surface water	0	[-]	S
Fraction of tonnage released to industrial soil	0	[-]	S
Fraction of tonnage released to agricultural soil	0	[-]	S
Fraction of the main local source	0.1	[-]	S
Number of emission days per year	240	[-]	S
Local emission to air during episode	7.407E+03	[kg.d-1]	S
Local emission to wastewater during episode	0.152	[kg.d-1]	O
Intermittent release	Yes		S
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
[2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29]			
Industry category	5 Personal / domestic use		S
Use category	29 Heat transferring agents		S
Fraction of tonnage for application	65	[%]	S
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
[PRIVATE USE]			
Use specific emission scenario	No		D
Emission tables	A4.1 (specific uses), B4.1 (general table)		S
Emission scenario	no special scenario selected/available		S
Fraction of tonnage released to air	0.95	[-]	S
Fraction of tonnage released to wastewater	5E-03	[-]	S
Fraction of tonnage released to surface water	0.015	[-]	S
Fraction of tonnage released to industrial soil	0.015	[-]	S
Fraction of tonnage released to agricultural soil	0.015	[-]	S
Fraction of the main local source	2E-03	[-]	O
Number of emission days per year	365	[-]	O
Local emission to air during episode	1	[kg.d-1]	S
Local emission to wastewater during episode	0.164	[kg.d-1]	O
Intermittent release	No		D
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
[3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29]			
Industry category	6 Public domain		S
Use category	29 Heat transferring agents		S
Fraction of tonnage for application	0.35	[-]	S

Name	Value	Units	Status
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
[INDUSTRIAL USE]			
Use specific emission scenario	No		D
Emission tables	A3.5 (specific uses), B3.3 (specific uses)		S
Emission scenario	no special scenario selected/available		S
Fraction of tonnage released to air	0.095	[-]	S
Fraction of tonnage released to wastewater	5E-03	[-]	S
Fraction of tonnage released to surface water	0.015	[-]	S
Fraction of tonnage released to industrial soil	0.015	[-]	S
Fraction of tonnage released to agricultural soil	0.015	[-]	S
Fraction of the main local source	2E-03	[-]	O
Number of emission days per year	50	[-]	O
Local emission to air during episode	10	[kg.d-1]	S
Local emission to wastewater during episode	0.642	[kg.d-1]	O
Intermittent release	No		D
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
TOTAL REGIONAL EMISSIONS TO COMPARTMENTS			
Total regional emission to air	2.3825E+04	[kg.d-1]	S
Total regional emission to wastewater	125	[kg.d-1]	S
Total regional emission to surface water	376	[kg.d-1]	S
Total regional emission to industrial soil	376	[kg.d-1]	S
Total regional emission to agricultural soil	376	[kg.d-1]	S
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
TOTAL CONTINENTAL EMISSIONS TO COMPARTMENTS			
Total continental emission to air	7.1475E+04	[kg.d-1]	S
Total continental emission to wastewater	376	[kg.d-1]	S
Total continental emission to surface water	1.129E+03	[kg.d-1]	S
Total continental emission to industrial soil	1.129E+03	[kg.d-1]	S
Total continental emission to agricultural soil	1.129E+03	[kg.d-1]	S
ENVIRONMENT-EXPOSURE			
PARTITION COEFFICIENTS			
Organic carbon-water partition coefficient	1	[l.kg-1]	S
ENVIRONMENT-EXPOSURE			
DEGRADATION AND TRANSFORMATION			
Characterization of biodegradability	Not biodegradable		S
Degradation calculation method in STP	First order, standard OECD/EU tests		D
Rate constant for biodegradation in STP	0	[d-1]	O
Rate constant for biodegradation in surface water	0	[d-1] (12[oC])	O
Rate constant for biodegradation in bulk soil	6.93E-07	[d-1] (12[oC])	O
Rate constant for biodegradation in aerated sediment	6.93E-07	[d-1] (12[oC])	O
Rate constant for hydrolysis in surface water	6.93E-07	[d-1] (12[oC])	O
Rate constant for photolysis in surface water	6.93E-07	[d-1]	O
ENVIRONMENT-EXPOSURE			
SEWAGE TREATMENT			
LOCAL STP [1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
OUTPUT			
Fraction of emission directed to air by STP	6.83E-03	[%]	O
Fraction of emission directed to water by STP	100	[%]	O
Fraction of emission directed to sludge by STP	0.0125	[%]	O
Fraction of the emission degraded in STP	0	[%]	O
Concentration in untreated wastewater	76	[ug.l-1]	O
Concentration of chemical (total) in the STP-effluent	0.076	[mg.l-1]	O
Concentration in effluent exceeds solubility	No		O
Concentration in dry sewage sludge	0.0241	[mg.kg-1]	O
PEC for micro-organisms in the STP	0.076	[mg.l-1]	O

Name	Value	Units	Status
ENVIRONMENT-EXPOSURE			
SEWAGE TREATMENT			
LOCAL STP [2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
OUTPUT			
Fraction of emission directed to air by STP	6.83E-03	[%]	O
Fraction of emission directed to water by STP	100	[%]	O
Fraction of emission directed to sludge by STP	0.0125	[%]	O
Fraction of the emission degraded in STP	0	[%]	O
Concentration in untreated wastewater	0.082	[mg.l-1]	O
Concentration of chemical (total) in the STP-effluent	0.082	[mg.l-1]	O
Concentration in effluent exceeds solubility	No		O
Concentration in dry sewage sludge	0.026	[mg.kg-1]	O
PEC for micro-organisms in the STP	0.082	[mg.l-1]	O
ENVIRONMENT-EXPOSURE			
SEWAGE TREATMENT			
LOCAL STP [3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
OUTPUT			
Fraction of emission directed to air by STP	6.83E-03	[%]	O
Fraction of emission directed to water by STP	100	[%]	O
Fraction of emission directed to sludge by STP	0.0125	[%]	O
Fraction of the emission degraded in STP	0	[%]	O
Concentration in untreated wastewater	0.321	[mg.l-1]	O
Concentration of chemical (total) in the STP-effluent	0.321	[mg.l-1]	O
Concentration in effluent exceeds solubility	No		O
Concentration in dry sewage sludge	0.102	[mg.kg-1]	O
PEC for micro-organisms in the STP	0.321	[mg.l-1]	O
ENVIRONMENT-EXPOSURE			
SEWAGE TREATMENT			
REGIONAL STP			
Fraction of emission directed to air	10	[%]	S
Fraction of emission directed to water	90	[%]	S
ENVIRONMENT-EXPOSURE			
SEWAGE TREATMENT			
CONTINENTAL STP			
Fraction of emission directed to air	10	[%]	S
Fraction of emission directed to water	90	[%]	S
Fraction of the emission degraded	0	[%]	S
ENVIRONMENT-EXPOSURE			
DISTRIBUTION			
LOCAL SCALE			
[1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
Concentration in air during emission episode	2.9E-08	[mg.m-3]	S
Annual average concentration in air, 100 m from point source	1.91E-08	[mg.m-3]	O
Concentration in surface water during emission episode (dissolved)	7.6E-03	[mg.l-1]	O
Annual average concentration in surface water (dissolved)	5E-03	[mg.l-1]	O
Local PEC in surface water during emission episode (dissolved)	7.93E-03	[mg.l-1]	O
Annual average local PEC in surface water (dissolved)	5.33E-03	[mg.l-1]	O
Local PEC in fresh-water sediment during emission episode	6.38E-03	[mg.kgwwt-1]	O
Concentration in seawater during emission episode (dissolved)	7.6E-04	[mg.l-1]	O
Annual average concentration in seawater (dissolved)	5E-04	[mg.l-1]	O
Local PEC in seawater during emission episode (dissolved)	9.6E-04	[mg.l-1]	O
Annual average local PEC in seawater (dissolved)	7E-04	[mg.l-1]	O
Local PEC in marine sediment during emission episode	7.72E-04	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 30 days	0.571	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 180 days	0.571	[mg.kgwwt-1]	O
Local PEC in grassland (total) averaged over 180 days	0.571	[mg.kgwwt-1]	O
Local PEC in groundwater under agricultural soil	4.22	[mg.l-1]	O

Name	Value	Units	Status
ENVIRONMENT-EXPOSURE			
DISTRIBUTION			
LOCAL SCALE			
[2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
Concentration in air during emission episode	2.78E-04	[mg.m-3]	O
Annual average concentration in air, 100 m from point source	2.78E-04	[mg.m-3]	O
Concentration in surface water during emission episode (dissolved)	8.2E-03	[mg.l-1]	O
Annual average concentration in surface water (dissolved)	8.2E-03	[mg.l-1]	O
Local PEC in surface water during emission episode (dissolved)	8.53E-03	[mg.l-1]	O
Annual average local PEC in surface water (dissolved)	8.53E-03	[mg.l-1]	O
Local PEC in fresh-water sediment during emission episode	6.86E-03	[mg.kgwwt-1]	O
Concentration in seawater during emission episode (dissolved)	8.2E-04	[mg.l-1]	O
Annual average concentration in seawater (dissolved)	8.2E-04	[mg.l-1]	O
Local PEC in seawater during emission episode (dissolved)	1.02E-03	[mg.l-1]	O
Annual average local PEC in seawater (dissolved)	1.02E-03	[mg.l-1]	O
Local PEC in marine sediment during emission episode	8.2E-04	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 30 days	5.15E-03	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 180 days	5.13E-03	[mg.kgwwt-1]	O
Local PEC in grassland (total) averaged over 180 days	5.12E-03	[mg.kgwwt-1]	O
Local PEC in groundwater under agricultural soil	0.0379	[mg.l-1]	O
ENVIRONMENT-EXPOSURE			
DISTRIBUTION			
LOCAL SCALE			
[3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
Concentration in air during emission episode	2.78E-03	[mg.m-3]	O
Annual average concentration in air, 100 m from point source	3.81E-04	[mg.m-3]	O
Concentration in surface water during emission episode (dissolved)	0.0321	[mg.l-1]	O
Annual average concentration in surface water (dissolved)	4.4E-03	[mg.l-1]	O
Local PEC in surface water during emission episode (dissolved)	0.0324	[mg.l-1]	O
Annual average local PEC in surface water (dissolved)	4.73E-03	[mg.l-1]	O
Local PEC in fresh-water sediment during emission episode	0.0261	[mg.kgwwt-1]	O
Concentration in seawater during emission episode (dissolved)	3.21E-03	[mg.l-1]	O
Annual average concentration in seawater (dissolved)	4.4E-04	[mg.l-1]	O
Local PEC in seawater during emission episode (dissolved)	3.41E-03	[mg.l-1]	O
Annual average local PEC in seawater (dissolved)	6.4E-04	[mg.l-1]	O
Local PEC in marine sediment during emission episode	2.74E-03	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 30 days	5.28E-03	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 180 days	5.22E-03	[mg.kgwwt-1]	O
Local PEC in grassland (total) averaged over 180 days	5.17E-03	[mg.kgwwt-1]	O
Local PEC in groundwater under agricultural soil	0.0386	[mg.l-1]	O
ENVIRONMENT-EXPOSURE			
DISTRIBUTION			
REGIONAL AND CONTINENTAL SCALE			
CONTINENTAL			
Continental PEC in surface water (dissolved)	3.5E-04	[mg.l-1]	O
Continental PEC in seawater (dissolved)	2.72E-04	[mg.l-1]	O
Continental PEC in air (total)	1.04E-03	[mg.m-3]	O
Continental PEC in agricultural soil (total)	1.16E-04	[mg.kgwwt-1]	O
Continental PEC in pore water of agricultural soils	8.51E-04	[mg.l-1]	O
Continental PEC in natural soil (total)	6.48E-05	[mg.kgwwt-1]	O
Continental PEC in industrial soil (total)	3.69E-04	[mg.kgwwt-1]	O
Continental PEC in sediment (total)	2.45E-04	[mg.kgwwt-1]	O
Continental PEC in seawater sediment (total)	1.94E-04	[mg.kgwwt-1]	O

Printed on	15-12-2017 16:53:50
Study	Trifluoroacetic acid
Substance	TFA 2025 mid EC50
Defaults	Standard Euses 2.1
Assessment types	1A, 1B, 2, 3A, 3B
Base set complete	No

Name	Value	Units	Status
ENVIRONMENT-EXPOSURE			
DISTRIBUTION			
REGIONAL AND CONTINENTAL SCALE			
REGIONAL			
Regional PEC in surface water (dissolved)	3.28E-04	[mg.l-1]	S
Regional PEC in seawater (dissolved)	2E-04	[mg.l-1]	S
Regional PEC in air (total)	4.1E-09	[mg.m-3]	S
Regional PEC in agricultural soil (total)	5E-03	[mg.kgwwt-1]	S
Regional PEC in pore water of agricultural soils	3.28E-04	[mg.l-1]	S
Regional PEC in natural soil (total)	5E-03	[mg.kgwwt-1]	S
Regional PEC in industrial soil (total)	5E-03	[mg.kgwwt-1]	S
Regional PEC in sediment (total)	5E-03	[mg.kgwwt-1]	S
Regional PEC in seawater sediment (total)	5E-03	[mg.kgwwt-1]	S
ENVIRONMENT-EXPOSURE			
BIOCONCENTRATION			
Bioconcentration factor for earthworms	0.848	[l.kgwwt-1]	O
Bioconcentration factor for fish	1.41	[l.kgwwt-1]	O
ENVIRONMENT-EXPOSURE			
SECONDARY POISONING [1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
Concentration in fish for secondary poisoning (freshwater)	3.99E-03	[mg.kgwwt-1]	O
Concentration in fish for secondary poisoning (marine)	6.36E-04	[mg.kgwwt-1]	O
Concentration in fish-eating marine top-predators	3.53E-04	[mg.kgwwt-1]	O
Concentration in earthworms from agricultural soil	1.64	[mg.kg-1]	O
ENVIRONMENT-EXPOSURE			
SECONDARY POISONING [2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
Concentration in fish for secondary poisoning (freshwater)	6.25E-03	[mg.kgwwt-1]	O
Concentration in fish for secondary poisoning (marine)	8.62E-04	[mg.kgwwt-1]	O
Concentration in fish-eating marine top-predators	3.98E-04	[mg.kgwwt-1]	O
Concentration in earthworms from agricultural soil	0.0151	[mg.kg-1]	O
ENVIRONMENT-EXPOSURE			
SECONDARY POISONING [3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
Concentration in fish for secondary poisoning (freshwater)	3.57E-03	[mg.kgwwt-1]	O
Concentration in fish for secondary poisoning (marine)	5.93E-04	[mg.kgwwt-1]	O
Concentration in fish-eating marine top-predators	3.45E-04	[mg.kgwwt-1]	O
Concentration in earthworms from agricultural soil	0.0153	[mg.kg-1]	O

Name	Value	Units	Status
ENVIRONMENT - EFFECTS			
MICRO-ORGANISMS			
Test system	Respiration inhibition, EU Annex V C.11, OECD 209 D		
EC50 for micro-organisms in a STP	832	[mg.l-1]	S
EC10 for micro-organisms in a STP	832	[mg.l-1]	S
NOEC for micro-organisms in a STP	832	[mg.l-1]	S
PNEC for micro-organisms in a STP	8.32	[mg.l-1]	O
Assessment factor applied in extrapolation to PNEC micro	10	[-]	S
ENVIRONMENT - EFFECTS			
FRESH_WATER ORGANISMS			
LC50 for fish	1.2E+03	[mg.l-1]	S
L(E)C50 for Daphnia	1.2E+03	[mg.l-1]	S
EC50 for algae	99	[mg.l-1]	S
LC50 for additional taxonomic group	??	[mg.l-1]	D
NOEC for fish	??	[mg.l-1]	D
NOEC for Daphnia	??	[mg.l-1]	D
NOEC for algae	??	[mg.l-1]	D
NOEC for additional taxonomic group	??	[mg.l-1]	D
PNEC for aquatic organisms	0.099	[mg.l-1]	O
PNEC for aquatic organisms, intermittent releases	0.99	[mg.l-1]	O
ENVIRONMENT - EFFECTS			
MARINE ORGANISMS			
LC50 for fish (marine)	??	[mg.l-1]	D
L(E)C50 for crustaceans (marine)	??	[mg.l-1]	D
EC50 for algae (marine)	103	[mg.l-1]	S
LC50 for additional taxonomic group (marine)	??	[mg.l-1]	D
NOEC for fish (marine)	??	[mg.l-1]	D
NOEC for crustaceans (marine)	??	[mg.l-1]	D
NOEC for algae (marine)	??	[mg.l-1]	D
NOEC for additional taxonomic group (marine)	??	[mg.l-1]	D
PNEC for marine organisms	9.9E-03	[mg.l-1]	O
ENVIRONMENT - EFFECTS			
FRESH-WATER SEDIMENT ORGANISMS			
LC50 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
PNEC for fresh-water sediment, normalised to 5% o.c. (regional)	0.0796	[mg.kgwwt-1]	O
ENVIRONMENT - EFFECTS			
MARINE SEDIMENT ORGANISMS			
LC50 for marine sediment organism	??	[mg.kgwwt-1]	D
EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D
PNEC for marine sediment, normalised to 5% o.c. (regional)	7.96E-03	[mg.kgwwt-1]	O

Name	Value	Units	Status
ENVIRONMENT - EFFECTS			
TERRESTRIAL ORGANISMS			
LC50 for plants	250	[mg.kgdwt-1]	S
LC50 for earthworms	??	[mg.kgwwt-1]	D
EC50 for microorganisms	??	[mg.kgwwt-1]	D
LC50 for other terrestrial species	??	[mg.kgwwt-1]	D
NOEC for plants	??	[mg.kgwwt-1]	D
NOEC for earthworms	??	[mg.kgwwt-1]	D
NOEC for microorganisms	??	[mg.kgwwt-1]	D
NOEC for additional taxonomic group	??	[mg.kgwwt-1]	D
NOEC for additional taxonomic group	??	[mg.kgwwt-1]	D
PNEC for terrestrial organisms	0.0134	[mg.kgwwt-1]	O
Equilibrium partitioning used for PNEC in soil?	Yes		O
ENVIRONMENT - EFFECTS			
BIRDS AND MAMMALS			
Oral NOAEL (repdose)	1E+03	[mg.kg-1.d-1]	S
NOEC via food (repdose)	1E+04	[mg.kg-1]	O
Inhalatory NOAEL (repdose)	1.75E+03	[mg.m-3]	O
Dermal NOAEL (repdose)	1E+03	[mg.kg-1.d-1]	O
Oral NOAEL (fert)	1E+03	[mg.kg-1.d-1]	S
NOEC via food (fert)	1E+04	[mg.kg-1]	O
Inhalatory NOAEL (fert)	1.75E+03	[mg.m-3]	O
Dermal NOAEL (fert)	1E+03	[mg.kg-1.d-1]	O
Oral NOAEL (mattox)	150	[mg.kg-1.d-1]	S
NOEC via food (mattox)	1.5E+03	[mg.kg-1]	O
Inhalatory NOAEL (mattox)	262	[mg.m-3]	O
Dermal NOAEL (mattox)	150	[mg.kg-1.d-1]	O
Oral NOAEL (devtox)	150	[mg.kg-1.d-1]	S
NOEC via food (devtox)	1.5E+03	[mg.kg-1]	O
Inhalatory NOAEL (devtox)	262	[mg.m-3]	O
Dermal NOAEL (devtox)	150	[mg.kg-1.d-1]	O
Duration of (sub-)chronic oral test	28 days		D
NOEC via food for secondary poisoning	1E+04	[mg.kg-1]	O
PNEC for secondary poisoning of birds and mammals	33.3	[mg.kg-1]	O

Name	Value	Units	Status
ENVIRONMENT - RISK CHARACTERIZATION			
LOCAL [1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
RCR for the local fresh-water compartment	8.01E-03	[-]	O
RCR for the local fresh-water compartment, statistical method	??	[-]	O
RCR for the local marine compartment	0.097	[-]	O
RCR for the local marine compartment, statistical method	??	[-]	O
RCR for the local fresh-water sediment compartment	0.0801	[-]	O
RCR for the local marine sediment compartment	0.097	[-]	O
RCR for the local soil compartment	42.6	[-]	O
RCR for the local soil compartment, statistical method	??	[-]	O
RCR for the sewage treatment plant	9.14E-03	[-]	O
RCR for fish-eating birds and mammals (fresh-water)	1.2E-04	[-]	O
RCR for fish-eating birds and mammals (marine)	1.91E-05	[-]	O
RCR for top predators (marine)	1.06E-05	[-]	O
RCR for worm-eating birds and mammals	0.0491	[-]	O
ENVIRONMENT - RISK CHARACTERIZATION			
LOCAL [2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
RCR for the local fresh-water compartment	0.0861	[-]	O
RCR for the local fresh-water compartment, statistical method	??	[-]	O
RCR for the local marine compartment	0.103	[-]	O
RCR for the local marine compartment, statistical method	??	[-]	O
RCR for the local fresh-water sediment compartment	0.0861	[-]	O
RCR for the local marine sediment compartment	0.103	[-]	O
RCR for the local soil compartment	0.384	[-]	O
RCR for the local soil compartment, statistical method	??	[-]	O
RCR for the sewage treatment plant	9.85E-03	[-]	O
RCR for fish-eating birds and mammals (fresh-water)	1.88E-04	[-]	O
RCR for fish-eating birds and mammals (marine)	2.58E-05	[-]	O
RCR for top predators (marine)	1.2E-05	[-]	O
RCR for worm-eating birds and mammals	4.52E-04	[-]	O
ENVIRONMENT - RISK CHARACTERIZATION			
LOCAL [3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
RCR for the local fresh-water compartment	0.328	[-]	O
RCR for the local fresh-water compartment, statistical method	??	[-]	O
RCR for the local marine compartment	0.345	[-]	O
RCR for the local marine compartment, statistical method	??	[-]	O
RCR for the local fresh-water sediment compartment	0.328	[-]	O
RCR for the local marine sediment compartment	0.345	[-]	O
RCR for the local soil compartment	0.395	[-]	O
RCR for the local soil compartment, statistical method	??	[-]	O
RCR for the sewage treatment plant	0.0386	[-]	O
RCR for fish-eating birds and mammals (fresh-water)	1.07E-04	[-]	O
RCR for fish-eating birds and mammals (marine)	1.78E-05	[-]	O
RCR for top predators (marine)	1.03E-05	[-]	O
RCR for worm-eating birds and mammals	4.6E-04	[-]	O
ENVIRONMENT - RISK CHARACTERIZATION			
REGIONAL			
RCR for the regional fresh-water compartment	3.31E-03	[-]	O
RCR for the regional fresh-water compartment, statistical method	??	[-]	O
RCR for the regional marine compartment	0.0202	[-]	O
RCR for the regional marine compartment, statistical method	??	[-]	O
RCR for the regional fresh-water sediment compartment	0.0628	[-]	O
RCR for the regional marine sediment compartment	0.628	[-]	O
RCR for the regional soil compartment	0.373	[-]	O
RCR for the regional soil compartment, statistical method	??	[-]	O

Name	Value	Units	Status
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
Purification factor for surface water	1	[-]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
CONCENTRATIONS IN INTAKE MEDIA [1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
Local concentration in wet fish	7.52E-03	[mg.kg-1]	O
Local concentration in root tissue of plant	3.96	[mg.kg-1]	O
Local concentration in leaves of plant	0.931	[mg.kg-1]	O
Local concentration in grass (wet weight)	0.931	[mg.kg-1]	O
Local concentration in drinking water	4.22	[mg.l-1]	O
Local concentration in meat (wet weight)	2.35E-04	[mg.kg-1]	O
Local concentration in milk (wet weight)	2.35E-03	[mg.kg-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
DOSES IN INTAKE MEDIA [1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
Daily dose through intake of drinking water	0.121	[mg.kg-1.d-1]	O
Daily dose through intake of fish	1.24E-05	[mg.kg-1.d-1]	O
Daily dose through intake of leaf crops	0.016	[mg.kg-1.d-1]	O
Daily dose through intake of root crops	0.0217	[mg.kg-1.d-1]	O
Daily dose through intake of meat	1.01E-06	[mg.kg-1.d-1]	O
Daily dose through intake of milk	1.88E-05	[mg.kg-1.d-1]	O
Daily dose through intake of air	6.62E-09	[mg.kg-1.d-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
FRACTIONS OF TOTAL DOSE [1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
Fraction of total dose through intake of drinking water	0.762	[-]	O
Fraction of total dose through intake of fish	7.81E-05	[-]	O
Fraction of total dose through intake of leaf crops	0.101	[-]	O
Fraction of total dose through intake of root crops	0.137	[-]	O
Fraction of total dose through intake of meat	6.37E-06	[-]	O
Fraction of total dose through intake of milk	1.19E-04	[-]	O
Fraction of total dose through intake of air	4.18E-08	[-]	O
Local total daily intake for humans	0.158	[mg.kg-1.d-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
CONCENTRATIONS IN INTAKE MEDIA [2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
Local concentration in wet fish	0.012	[mg.kg-1]	O
Local concentration in root tissue of plant	0.0356	[mg.kg-1]	O
Local concentration in leaves of plant	0.177	[mg.kg-1]	O
Local concentration in grass (wet weight)	0.177	[mg.kg-1]	O
Local concentration in drinking water	0.0379	[mg.l-1]	O
Local concentration in meat (wet weight)	1.12E-05	[mg.kg-1]	O
Local concentration in milk (wet weight)	1.12E-04	[mg.kg-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
DOSES IN INTAKE MEDIA [2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
Daily dose through intake of drinking water	1.08E-03	[mg.kg-1.d-1]	O
Daily dose through intake of fish	1.98E-05	[mg.kg-1.d-1]	O
Daily dose through intake of leaf crops	3.03E-03	[mg.kg-1.d-1]	O
Daily dose through intake of root crops	1.95E-04	[mg.kg-1.d-1]	O
Daily dose through intake of meat	4.81E-08	[mg.kg-1.d-1]	O
Daily dose through intake of milk	8.96E-07	[mg.kg-1.d-1]	O
Daily dose through intake of air	7.94E-05	[mg.kg-1.d-1]	O

Name	Value	Units	Status
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
FRACTIONS OF TOTAL DOSE [2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
Fraction of total dose through intake of drinking water	0.246	[-]	O
Fraction of total dose through intake of fish	4.49E-03	[-]	O
Fraction of total dose through intake of leaf crops	0.687	[-]	O
Fraction of total dose through intake of root crops	0.0442	[-]	O
Fraction of total dose through intake of meat	1.09E-05	[-]	O
Fraction of total dose through intake of milk	2.03E-04	[-]	O
Fraction of total dose through intake of air	0.018	[-]	O
Local total daily intake for humans	4.41E-03	[mg.kg-1.d-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
CONCENTRATIONS IN INTAKE MEDIA [3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
Local concentration in wet fish	6.68E-03	[mg.kg-1]	O
Local concentration in root tissue of plant	0.0362	[mg.kg-1]	O
Local concentration in leaves of plant	0.239	[mg.kg-1]	O
Local concentration in grass (wet weight)	0.239	[mg.kg-1]	O
Local concentration in drinking water	0.0386	[mg.l-1]	O
Local concentration in meat (wet weight)	1.46E-05	[mg.kg-1]	O
Local concentration in milk (wet weight)	1.46E-04	[mg.kg-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
DOSES IN INTAKE MEDIA [3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
Daily dose through intake of drinking water	1.1E-03	[mg.kg-1.d-1]	O
Daily dose through intake of fish	1.1E-05	[mg.kg-1.d-1]	O
Daily dose through intake of leaf crops	4.1E-03	[mg.kg-1.d-1]	O
Daily dose through intake of root crops	1.98E-04	[mg.kg-1.d-1]	O
Daily dose through intake of meat	6.27E-08	[mg.kg-1.d-1]	O
Daily dose through intake of milk	1.17E-06	[mg.kg-1.d-1]	O
Daily dose through intake of air	1.09E-04	[mg.kg-1.d-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
FRACTIONS OF TOTAL DOSE [3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
Fraction of total dose through intake of drinking water	0.2	[-]	O
Fraction of total dose through intake of fish	1.99E-03	[-]	O
Fraction of total dose through intake of leaf crops	0.743	[-]	O
Fraction of total dose through intake of root crops	0.0359	[-]	O
Fraction of total dose through intake of meat	1.13E-05	[-]	O
Fraction of total dose through intake of milk	2.11E-04	[-]	O
Fraction of total dose through intake of air	0.0197	[-]	O
Local total daily intake for humans	5.52E-03	[mg.kg-1.d-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
REGIONAL SCALE			
CONCENTRATIONS IN INTAKE MEDIA			
Regional concentration in wet fish	4.63E-04	[mg.kg-1]	O
Regional concentration in root tissue of plant	3.08E-04	[mg.kg-1]	O
Regional concentration in leaves of plant	7.48E-05	[mg.kg-1]	O
Regional concentration in grass (wet weight)	7.48E-05	[mg.kg-1]	O
Regional concentration in drinking water	1.23E-04	[mg.l-1]	S
Regional concentration in meat (wet weight)	1.12E-08	[mg.kg-1]	O
Regional concentration in milk (wet weight)	1.12E-07	[mg.kg-1]	O

Name	Value	Units	Status
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
REGIONAL SCALE			
DOSES IN INTAKE MEDIA			
Daily dose through intake of drinking water	3.51E-06	[mg.kg-1.d-1]	O
Daily dose through intake of fish	7.61E-07	[mg.kg-1.d-1]	O
Daily dose through intake of leaf crops	1.28E-06	[mg.kg-1.d-1]	O
Daily dose through intake of root crops	1.69E-06	[mg.kg-1.d-1]	O
Daily dose through intake of meat	4.83E-11	[mg.kg-1.d-1]	O
Daily dose through intake of milk	9.01E-10	[mg.kg-1.d-1]	O
Daily dose through intake of air	1.17E-09	[mg.kg-1.d-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
REGIONAL SCALE			
FRACTIONS OF TOTAL DOSE			
Fraction of total dose through intake of drinking water	0.485	[-]	O
Fraction of total dose through intake of fish	0.105	[-]	O
Fraction of total dose through intake of leaf crops	0.177	[-]	O
Fraction of total dose through intake of root crops	0.233	[-]	O
Fraction of total dose through intake of meat	6.67E-06	[-]	O
Fraction of total dose through intake of milk	1.24E-04	[-]	O
Fraction of total dose through intake of air	1.62E-04	[-]	O
Regional total daily intake for humans	7.25E-06	[mg.kg-1.d-1]	O

Name	Value	Units	Status
HUMAN HEALTH - RISK CHARACTERIZATION			
CURRENT CLASSIFICATION			
Corrosive (C, R34 or R35)	Yes		S
Irritating to skin (Xi, R38)	No		D
Irritating to eyes (Xi, R36)	No		D
Risk of serious damage to eyes (Xi, R41)	No		D
Irritating to respiratory system (Xi, R37)	No		D
May cause sensitisation by inhalation (Xn, R42)	No		D
May cause sensitisation by skin contact (Xi, R43)	No		D
May cause cancer (T, R45)	No		D
May cause cancer by inhalation (T, R49)	No		D
Possible risk of irreversible effects (Xn, R40)	No		D
HUMAN HEALTH - RISK CHARACTERIZATION			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL [1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
MOS, local, inhalatory (repdose)	7.55E+10	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (repdose)	7.55E+10	[-]	O
MOS, local, total exposure (repdose)	6.32E+03	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (repdose)	6.32E+03	[-]	O
MOS, local, inhalatory (fert)	7.55E+10	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (fert)	7.55E+10	[-]	O
MOS, local, total exposure (fert)	6.32E+03	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (fert)	6.32E+03	[-]	O
MOS, local, inhalatory (mattox)	1.13E+10	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (mattox)	1.13E+10	[-]	O
MOS, local, total exposure (mattox)	947	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (mattox)	947	[-]	O
MOS, local, inhalatory (devtox)	1.13E+10	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (devtox)	1.13E+10	[-]	O
MOS, local, total exposure (devtox)	947	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (devtox)	947	[-]	O
HUMAN HEALTH - RISK CHARACTERIZATION			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL [2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
MOS, local, inhalatory (repdose)	6.29E+06	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (repdose)	6.29E+06	[-]	O
MOS, local, total exposure (repdose)	2.27E+05	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (repdose)	2.27E+05	[-]	O
MOS, local, inhalatory (fert)	6.29E+06	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (fert)	6.29E+06	[-]	O
MOS, local, total exposure (fert)	2.27E+05	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (fert)	2.27E+05	[-]	O
MOS, local, inhalatory (mattox)	9.44E+05	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (mattox)	9.44E+05	[-]	O
MOS, local, total exposure (mattox)	3.4E+04	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (mattox)	3.4E+04	[-]	O
MOS, local, inhalatory (devtox)	9.44E+05	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (devtox)	9.44E+05	[-]	O
MOS, local, total exposure (devtox)	3.4E+04	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (devtox)	3.4E+04	[-]	O

Name	Value	Units	Status
HUMAN HEALTH - RISK CHARACTERIZATION			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL [3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
MOS, local, inhalatory (repdose)	4.6E+06	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (repdose)	4.6E+06	[-]	O
MOS, local, total exposure (repdose)	1.81E+05	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (repdose)	1.81E+05	[-]	O
MOS, local, inhalatory (fert)	4.6E+06	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (fert)	4.6E+06	[-]	O
MOS, local, total exposure (fert)	1.81E+05	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (fert)	1.81E+05	[-]	O
MOS, local, inhalatory (mattox)	6.89E+05	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (mattox)	6.89E+05	[-]	O
MOS, local, total exposure (mattox)	2.72E+04	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (mattox)	2.72E+04	[-]	O
MOS, local, inhalatory (devtox)	6.89E+05	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (devtox)	6.89E+05	[-]	O
MOS, local, total exposure (devtox)	2.72E+04	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (devtox)	2.72E+04	[-]	O
HUMAN HEALTH - RISK CHARACTERIZATION			
HUMANS EXPOSED VIA THE ENVIRONMENT			
REGIONAL			
MOS, regional, inhalatory (repdose)	4.27E+11	[-]	O
Ratio MOS/Ref-MOS, regional, inhalatory (repdose)	4.27E+11	[-]	O
MOS, regional, total exposure (repdose)	1.38E+08	[-]	O
Ratio MOS/Ref-MOS, regional, total exposure (repdose)	1.38E+08	[-]	O
MOS, regional, inhalatory (fert)	4.27E+11	[-]	O
Ratio MOS/Ref-MOS, regional, inhalatory (fert)	4.27E+11	[-]	O
MOS, regional, total exposure (fert)	1.38E+08	[-]	O
Ratio MOS/Ref-MOS, regional, total exposure (fert)	1.38E+08	[-]	O
MOS, regional, inhalatory (mattox)	6.4E+10	[-]	O
Ratio MOS/Ref-MOS, regional, inhalatory (mattox)	6.4E+10	[-]	O
MOS, regional, total exposure (mattox)	2.07E+07	[-]	O
Ratio MOS/Ref-MOS, regional, total exposure (mattox)	2.07E+07	[-]	O
MOS, regional, inhalatory (devtox)	6.4E+10	[-]	O
Ratio MOS/Ref-MOS, regional, inhalatory (devtox)	6.4E+10	[-]	O
MOS, regional, total exposure (devtox)	2.07E+07	[-]	O
Ratio MOS/Ref-MOS, regional, total exposure (devtox)	2.07E+07	[-]	O

EUSES 2 Summary report	Single substance
Printed on	15-12-2017 16:58:29
Study	TFA 2025 high EC50
Substance	Trifluoroacetic acid
Defaults	Standard Euses 2.1
Assessment types	1A, 1B, 2, 3A, 3B
Base set complete	No
Explanation status column	O = Output; D = Default; S = Set; I = Imported

Name	Value	Units	Status
IDENTIFICATION OF THE SUBSTANCE			
General name	Trifluoroacetic acid		S
CAS-No	76-05-1		S
EC-notification no.	200-929-3		S
EINECS no.	200-929-3		S
Molecular weight	114.02	[g.mol-1]	S

Printed on	15-12-2017 16:58:29
Study	Trifluoroacetic acid
Substance	TFA 2025 high EC50
Defaults	Standard Euses 2.1
Assessment types	1A, 1B, 2, 3A, 3B
Base set complete	No

Name	Value	Units	Status
PHYSICO-CHEMICAL PROPERTIES			
Melting point	-15.2	[oC]	S
Boiling point	71.78	[oC]	S
Vapour pressure at test temperature	1.58E+04	[Pa]	S
Vapour pressure at 25 [oC]	1.58E+04	[Pa]	O
Water solubility at test temperature	1E+05	[mg.l-1]	S
Water solubility at 25 [oC]	1E+05	[mg.l-1]	O
Octanol-water partition coefficient	-0.2	[log10]	S
Henry's law constant at 25 [oC]	7.13E-03	[Pa.m3.mol-1]	S

Name	Value	Units	Status
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
Tonnage of substance in Europe	2E+04	[tonnes.yr-1]	O
Regional production volume of substance	2E+04	[tonnes.yr-1]	O
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
[1 "CHEMICAL PRODUCTION", IC=3/UC=29]			
Industry category	3 Chemical industry: chemicals used in synthesis		S
Use category	29 Heat transferring agents		S
Fraction of tonnage for application	100	[%]	O
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
[PRODUCTION]			
Use specific emission scenario	No		D
Emission tables	A1.1 (general table), B1.6 (general table)		S
Emission scenario	no special scenario selected/available		S
Main category production	Ib Intermed. stored on-site/continuous prod.		S
Fraction of tonnage released to air	1	[-]	S
Fraction of tonnage released to wastewater	0	[-]	S
Fraction of tonnage released to surface water	0	[-]	S
Fraction of tonnage released to industrial soil	0	[-]	S
Fraction of tonnage released to agricultural soil	0	[-]	S
Fraction of the main local source	0.1	[-]	S
Number of emission days per year	240	[-]	S
Local emission to air during episode	7.407E+03	[kg.d-1]	S
Local emission to wastewater during episode	0.152	[kg.d-1]	O
Intermittent release	Yes		S
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
[2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29]			
Industry category	5 Personal / domestic use		S
Use category	29 Heat transferring agents		S
Fraction of tonnage for application	65	[%]	S
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
[PRIVATE USE]			
Use specific emission scenario	No		D
Emission tables	A4.1 (specific uses), B4.1 (general table)		S
Emission scenario	no special scenario selected/available		S
Fraction of tonnage released to air	0.95	[-]	S
Fraction of tonnage released to wastewater	5E-03	[-]	S
Fraction of tonnage released to surface water	0.015	[-]	S
Fraction of tonnage released to industrial soil	0.015	[-]	S
Fraction of tonnage released to agricultural soil	0.015	[-]	S
Fraction of the main local source	2E-03	[-]	O
Number of emission days per year	365	[-]	O
Local emission to air during episode	1	[kg.d-1]	S
Local emission to wastewater during episode	0.164	[kg.d-1]	O
Intermittent release	No		D
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
[3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29]			
Industry category	6 Public domain		S
Use category	29 Heat transferring agents		S
Fraction of tonnage for application	0.35	[-]	S

Printed on	15-12-2017 16:58:29
Study	Trifluoroacetic acid
Substance	TFA 2025 high EC50
Defaults	Standard Euses 2.1
Assessment types	1A, 1B, 2, 3A, 3B
Base set complete	No

Name	Value	Units	Status
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
[INDUSTRIAL USE]			
Use specific emission scenario	No		D
Emission tables	A3.5 (specific uses), B3.3 (specific uses)		S
Emission scenario	no special scenario selected/available		S
Fraction of tonnage released to air	0.095	[-]	S
Fraction of tonnage released to wastewater	5E-03	[-]	S
Fraction of tonnage released to surface water	0.015	[-]	S
Fraction of tonnage released to industrial soil	0.015	[-]	S
Fraction of tonnage released to agricultural soil	0.015	[-]	S
Fraction of the main local source	2E-03	[-]	O
Number of emission days per year	50	[-]	O
Local emission to air during episode	10	[kg.d-1]	S
Local emission to wastewater during episode	0.642	[kg.d-1]	O
Intermittent release	No		D
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
TOTAL REGIONAL EMISSIONS TO COMPARTMENTS			
Total regional emission to air	2.3825E+04	[kg.d-1]	S
Total regional emission to wastewater	125	[kg.d-1]	S
Total regional emission to surface water	376	[kg.d-1]	S
Total regional emission to industrial soil	376	[kg.d-1]	S
Total regional emission to agricultural soil	376	[kg.d-1]	S
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
TOTAL CONTINENTAL EMISSIONS TO COMPARTMENTS			
Total continental emission to air	7.1475E+04	[kg.d-1]	S
Total continental emission to wastewater	376	[kg.d-1]	S
Total continental emission to surface water	1.129E+03	[kg.d-1]	S
Total continental emission to industrial soil	1.129E+03	[kg.d-1]	S
Total continental emission to agricultural soil	1.129E+03	[kg.d-1]	S
ENVIRONMENT-EXPOSURE			
PARTITION COEFFICIENTS			
Organic carbon-water partition coefficient	1	[l.kg-1]	S
ENVIRONMENT-EXPOSURE			
DEGRADATION AND TRANSFORMATION			
Characterization of biodegradability	Not biodegradable		S
Degradation calculation method in STP	First order, standard OECD/EU tests		D
Rate constant for biodegradation in STP	0	[d-1]	O
Rate constant for biodegradation in surface water	0	[d-1] (12[oC])	O
Rate constant for biodegradation in bulk soil	6.93E-07	[d-1] (12[oC])	O
Rate constant for biodegradation in aerated sediment	6.93E-07	[d-1] (12[oC])	O
Rate constant for hydrolysis in surface water	6.93E-07	[d-1] (12[oC])	O
Rate constant for photolysis in surface water	6.93E-07	[d-1]	O
ENVIRONMENT-EXPOSURE			
SEWAGE TREATMENT			
LOCAL STP [1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
OUTPUT			
Fraction of emission directed to air by STP	6.83E-03	[%]	O
Fraction of emission directed to water by STP	100	[%]	O
Fraction of emission directed to sludge by STP	0.0125	[%]	O
Fraction of the emission degraded in STP	0	[%]	O
Concentration in untreated wastewater	76	[ug.l-1]	O
Concentration of chemical (total) in the STP-effluent	0.076	[mg.l-1]	O
Concentration in effluent exceeds solubility	No		O
Concentration in dry sewage sludge	0.0241	[mg.kg-1]	O
PEC for micro-organisms in the STP	0.076	[mg.l-1]	O

Name	Value	Units	Status
ENVIRONMENT-EXPOSURE			
SEWAGE TREATMENT			
LOCAL STP [2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
OUTPUT			
Fraction of emission directed to air by STP	6.83E-03	[%]	O
Fraction of emission directed to water by STP	100	[%]	O
Fraction of emission directed to sludge by STP	0.0125	[%]	O
Fraction of the emission degraded in STP	0	[%]	O
Concentration in untreated wastewater	0.082	[mg.l-1]	O
Concentration of chemical (total) in the STP-effluent	0.082	[mg.l-1]	O
Concentration in effluent exceeds solubility	No		O
Concentration in dry sewage sludge	0.026	[mg.kg-1]	O
PEC for micro-organisms in the STP	0.082	[mg.l-1]	O
ENVIRONMENT-EXPOSURE			
SEWAGE TREATMENT			
LOCAL STP [3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
OUTPUT			
Fraction of emission directed to air by STP	6.83E-03	[%]	O
Fraction of emission directed to water by STP	100	[%]	O
Fraction of emission directed to sludge by STP	0.0125	[%]	O
Fraction of the emission degraded in STP	0	[%]	O
Concentration in untreated wastewater	0.321	[mg.l-1]	O
Concentration of chemical (total) in the STP-effluent	0.321	[mg.l-1]	O
Concentration in effluent exceeds solubility	No		O
Concentration in dry sewage sludge	0.102	[mg.kg-1]	O
PEC for micro-organisms in the STP	0.321	[mg.l-1]	O
ENVIRONMENT-EXPOSURE			
SEWAGE TREATMENT			
REGIONAL STP			
Fraction of emission directed to air	10	[%]	S
Fraction of emission directed to water	90	[%]	S
ENVIRONMENT-EXPOSURE			
SEWAGE TREATMENT			
CONTINENTAL STP			
Fraction of emission directed to air	10	[%]	S
Fraction of emission directed to water	90	[%]	S
Fraction of the emission degraded	0	[%]	S
ENVIRONMENT-EXPOSURE			
DISTRIBUTION			
LOCAL SCALE			
[1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
Concentration in air during emission episode	2.9E-08	[mg.m-3]	S
Annual average concentration in air, 100 m from point source	1.91E-08	[mg.m-3]	O
Concentration in surface water during emission episode (dissolved)	7.6E-03	[mg.l-1]	O
Annual average concentration in surface water (dissolved)	5E-03	[mg.l-1]	O
Local PEC in surface water during emission episode (dissolved)	7.93E-03	[mg.l-1]	O
Annual average local PEC in surface water (dissolved)	5.33E-03	[mg.l-1]	O
Local PEC in fresh-water sediment during emission episode	6.38E-03	[mg.kgwwt-1]	O
Concentration in seawater during emission episode (dissolved)	7.6E-04	[mg.l-1]	O
Annual average concentration in seawater (dissolved)	5E-04	[mg.l-1]	O
Local PEC in seawater during emission episode (dissolved)	9.6E-04	[mg.l-1]	O
Annual average local PEC in seawater (dissolved)	7E-04	[mg.l-1]	O
Local PEC in marine sediment during emission episode	7.72E-04	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 30 days	0.571	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 180 days	0.571	[mg.kgwwt-1]	O
Local PEC in grassland (total) averaged over 180 days	0.571	[mg.kgwwt-1]	O
Local PEC in groundwater under agricultural soil	4.22	[mg.l-1]	O

Name	Value	Units	Status
ENVIRONMENT-EXPOSURE			
DISTRIBUTION			
LOCAL SCALE			
[2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
Concentration in air during emission episode	2.78E-04	[mg.m-3]	O
Annual average concentration in air, 100 m from point source	2.78E-04	[mg.m-3]	O
Concentration in surface water during emission episode (dissolved)	8.2E-03	[mg.l-1]	O
Annual average concentration in surface water (dissolved)	8.2E-03	[mg.l-1]	O
Local PEC in surface water during emission episode (dissolved)	8.53E-03	[mg.l-1]	O
Annual average local PEC in surface water (dissolved)	8.53E-03	[mg.l-1]	O
Local PEC in fresh-water sediment during emission episode	6.86E-03	[mg.kgwwt-1]	O
Concentration in seawater during emission episode (dissolved)	8.2E-04	[mg.l-1]	O
Annual average concentration in seawater (dissolved)	8.2E-04	[mg.l-1]	O
Local PEC in seawater during emission episode (dissolved)	1.02E-03	[mg.l-1]	O
Annual average local PEC in seawater (dissolved)	1.02E-03	[mg.l-1]	O
Local PEC in marine sediment during emission episode	8.2E-04	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 30 days	5.15E-03	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 180 days	5.13E-03	[mg.kgwwt-1]	O
Local PEC in grassland (total) averaged over 180 days	5.12E-03	[mg.kgwwt-1]	O
Local PEC in groundwater under agricultural soil	0.0379	[mg.l-1]	O
ENVIRONMENT-EXPOSURE			
DISTRIBUTION			
LOCAL SCALE			
[3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
Concentration in air during emission episode	2.78E-03	[mg.m-3]	O
Annual average concentration in air, 100 m from point source	3.81E-04	[mg.m-3]	O
Concentration in surface water during emission episode (dissolved)	0.0321	[mg.l-1]	O
Annual average concentration in surface water (dissolved)	4.4E-03	[mg.l-1]	O
Local PEC in surface water during emission episode (dissolved)	0.0324	[mg.l-1]	O
Annual average local PEC in surface water (dissolved)	4.73E-03	[mg.l-1]	O
Local PEC in fresh-water sediment during emission episode	0.0261	[mg.kgwwt-1]	O
Concentration in seawater during emission episode (dissolved)	3.21E-03	[mg.l-1]	O
Annual average concentration in seawater (dissolved)	4.4E-04	[mg.l-1]	O
Local PEC in seawater during emission episode (dissolved)	3.41E-03	[mg.l-1]	O
Annual average local PEC in seawater (dissolved)	6.4E-04	[mg.l-1]	O
Local PEC in marine sediment during emission episode	2.74E-03	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 30 days	5.28E-03	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 180 days	5.22E-03	[mg.kgwwt-1]	O
Local PEC in grassland (total) averaged over 180 days	5.17E-03	[mg.kgwwt-1]	O
Local PEC in groundwater under agricultural soil	0.0386	[mg.l-1]	O
ENVIRONMENT-EXPOSURE			
DISTRIBUTION			
REGIONAL AND CONTINENTAL SCALE			
CONTINENTAL			
Continental PEC in surface water (dissolved)	3.5E-04	[mg.l-1]	O
Continental PEC in seawater (dissolved)	2.72E-04	[mg.l-1]	O
Continental PEC in air (total)	1.04E-03	[mg.m-3]	O
Continental PEC in agricultural soil (total)	1.16E-04	[mg.kgwwt-1]	O
Continental PEC in pore water of agricultural soils	8.51E-04	[mg.l-1]	O
Continental PEC in natural soil (total)	6.48E-05	[mg.kgwwt-1]	O
Continental PEC in industrial soil (total)	3.69E-04	[mg.kgwwt-1]	O
Continental PEC in sediment (total)	2.45E-04	[mg.kgwwt-1]	O
Continental PEC in seawater sediment (total)	1.94E-04	[mg.kgwwt-1]	O

Name	Value	Units	Status
ENVIRONMENT-EXPOSURE			
DISTRIBUTION			
REGIONAL AND CONTINENTAL SCALE			
REGIONAL			
Regional PEC in surface water (dissolved)	3.28E-04	[mg.l-1]	S
Regional PEC in seawater (dissolved)	2E-04	[mg.l-1]	S
Regional PEC in air (total)	4.1E-09	[mg.m-3]	S
Regional PEC in agricultural soil (total)	5E-03	[mg.kgwwt-1]	S
Regional PEC in pore water of agricultural soils	3.28E-04	[mg.l-1]	S
Regional PEC in natural soil (total)	5E-03	[mg.kgwwt-1]	S
Regional PEC in industrial soil (total)	5E-03	[mg.kgwwt-1]	S
Regional PEC in sediment (total)	5E-03	[mg.kgwwt-1]	S
Regional PEC in seawater sediment (total)	5E-03	[mg.kgwwt-1]	S
ENVIRONMENT-EXPOSURE			
BIOCONCENTRATION			
Bioconcentration factor for earthworms	0.848	[l.kgwwt-1]	O
Bioconcentration factor for fish	1.41	[l.kgwwt-1]	O
ENVIRONMENT-EXPOSURE			
SECONDARY POISONING [1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
Concentration in fish for secondary poisoning (freshwater)	3.99E-03	[mg.kgwwt-1]	O
Concentration in fish for secondary poisoning (marine)	6.36E-04	[mg.kgwwt-1]	O
Concentration in fish-eating marine top-predators	3.53E-04	[mg.kgwwt-1]	O
Concentration in earthworms from agricultural soil	1.64	[mg.kg-1]	O
ENVIRONMENT-EXPOSURE			
SECONDARY POISONING [2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
Concentration in fish for secondary poisoning (freshwater)	6.25E-03	[mg.kgwwt-1]	O
Concentration in fish for secondary poisoning (marine)	8.62E-04	[mg.kgwwt-1]	O
Concentration in fish-eating marine top-predators	3.98E-04	[mg.kgwwt-1]	O
Concentration in earthworms from agricultural soil	0.0151	[mg.kg-1]	O
ENVIRONMENT-EXPOSURE			
SECONDARY POISONING [3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
Concentration in fish for secondary poisoning (freshwater)	3.57E-03	[mg.kgwwt-1]	O
Concentration in fish for secondary poisoning (marine)	5.93E-04	[mg.kgwwt-1]	O
Concentration in fish-eating marine top-predators	3.45E-04	[mg.kgwwt-1]	O
Concentration in earthworms from agricultural soil	0.0153	[mg.kg-1]	O

Name	Value	Units	Status
ENVIRONMENT - EFFECTS			
MICRO-ORGANISMS			
Test system	Respiration inhibition, EU Annex V C.11, OECD 209 D		
EC50 for micro-organisms in a STP	832	[mg.l-1]	S
EC10 for micro-organisms in a STP	832	[mg.l-1]	S
NOEC for micro-organisms in a STP	832	[mg.l-1]	S
PNEC for micro-organisms in a STP	8.32	[mg.l-1]	O
Assessment factor applied in extrapolation to PNEC micro	10	[-]	S
ENVIRONMENT - EFFECTS			
FRESH_WATER ORGANISMS			
LC50 for fish	1.2E+03	[mg.l-1]	S
L(E)C50 for Daphnia	1.2E+03	[mg.l-1]	S
EC50 for algae	441	[mg.l-1]	S
LC50 for additional taxonomic group	??	[mg.l-1]	D
NOEC for fish	??	[mg.l-1]	D
NOEC for Daphnia	??	[mg.l-1]	D
NOEC for algae	??	[mg.l-1]	D
NOEC for additional taxonomic group	??	[mg.l-1]	D
PNEC for aquatic organisms	0.441	[mg.l-1]	O
PNEC for aquatic organisms, intermittent releases	4.41	[mg.l-1]	O
ENVIRONMENT - EFFECTS			
MARINE ORGANISMS			
LC50 for fish (marine)	??	[mg.l-1]	D
L(E)C50 for crustaceans (marine)	??	[mg.l-1]	D
EC50 for algae (marine)	732	[mg.l-1]	S
LC50 for additional taxonomic group (marine)	??	[mg.l-1]	D
NOEC for fish (marine)	??	[mg.l-1]	D
NOEC for crustaceans (marine)	??	[mg.l-1]	D
NOEC for algae (marine)	??	[mg.l-1]	D
NOEC for additional taxonomic group (marine)	??	[mg.l-1]	D
PNEC for marine organisms	0.0441	[mg.l-1]	O
ENVIRONMENT - EFFECTS			
FRESH-WATER SEDIMENT ORGANISMS			
LC50 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
PNEC for fresh-water sediment, normalised to 5% o.c. (regional)	0.355	[mg.kgwwt-1]	O
ENVIRONMENT - EFFECTS			
MARINE SEDIMENT ORGANISMS			
LC50 for marine sediment organism	??	[mg.kgwwt-1]	D
EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D
PNEC for marine sediment, normalised to 5% o.c. (regional)	0.0355	[mg.kgwwt-1]	O

Name	Value	Units	Status
ENVIRONMENT - EFFECTS			
TERRESTRIAL ORGANISMS			
LC50 for plants	250	[mg.kgdwt-1]	S
LC50 for earthworms	??	[mg.kgwwt-1]	D
EC50 for microorganisms	??	[mg.kgwwt-1]	D
LC50 for other terrestrial species	??	[mg.kgwwt-1]	D
NOEC for plants	??	[mg.kgwwt-1]	D
NOEC for earthworms	??	[mg.kgwwt-1]	D
NOEC for microorganisms	??	[mg.kgwwt-1]	D
NOEC for additional taxonomic group	??	[mg.kgwwt-1]	D
NOEC for additional taxonomic group	??	[mg.kgwwt-1]	D
PNEC for terrestrial organisms	0.0597	[mg.kgwwt-1]	O
Equilibrium partitioning used for PNEC in soil?	Yes		O
ENVIRONMENT - EFFECTS			
BIRDS AND MAMMALS			
Oral NOAEL (repdose)	1E+03	[mg.kg-1.d-1]	S
NOEC via food (repdose)	1E+04	[mg.kg-1]	O
Inhalatory NOAEL (repdose)	1.75E+03	[mg.m-3]	O
Dermal NOAEL (repdose)	1E+03	[mg.kg-1.d-1]	O
Oral NOAEL (fert)	1E+03	[mg.kg-1.d-1]	S
NOEC via food (fert)	1E+04	[mg.kg-1]	O
Inhalatory NOAEL (fert)	1.75E+03	[mg.m-3]	O
Dermal NOAEL (fert)	1E+03	[mg.kg-1.d-1]	O
Oral NOAEL (mattox)	150	[mg.kg-1.d-1]	S
NOEC via food (mattox)	1.5E+03	[mg.kg-1]	O
Inhalatory NOAEL (mattox)	262	[mg.m-3]	O
Dermal NOAEL (mattox)	150	[mg.kg-1.d-1]	O
Oral NOAEL (devtox)	150	[mg.kg-1.d-1]	S
NOEC via food (devtox)	1.5E+03	[mg.kg-1]	O
Inhalatory NOAEL (devtox)	262	[mg.m-3]	O
Dermal NOAEL (devtox)	150	[mg.kg-1.d-1]	O
Duration of (sub-)chronic oral test	28 days		D
NOEC via food for secondary poisoning	1E+04	[mg.kg-1]	O
PNEC for secondary poisoning of birds and mammals	33.3	[mg.kg-1]	O

Name	Value	Units	Status
ENVIRONMENT - RISK CHARACTERIZATION			
LOCAL [1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
RCR for the local fresh-water compartment	1.8E-03	[-]	O
RCR for the local fresh-water compartment, statistical method	??	[-]	O
RCR for the local marine compartment	0.0218	[-]	O
RCR for the local marine compartment, statistical method	??	[-]	O
RCR for the local fresh-water sediment compartment	0.018	[-]	O
RCR for the local marine sediment compartment	0.0218	[-]	O
RCR for the local soil compartment	9.57	[-]	O
RCR for the local soil compartment, statistical method	??	[-]	O
RCR for the sewage treatment plant	9.14E-03	[-]	O
RCR for fish-eating birds and mammals (fresh-water)	1.2E-04	[-]	O
RCR for fish-eating birds and mammals (marine)	1.91E-05	[-]	O
RCR for top predators (marine)	1.06E-05	[-]	O
RCR for worm-eating birds and mammals	0.0491	[-]	O
ENVIRONMENT - RISK CHARACTERIZATION			
LOCAL [2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
RCR for the local fresh-water compartment	0.0193	[-]	O
RCR for the local fresh-water compartment, statistical method	??	[-]	O
RCR for the local marine compartment	0.0231	[-]	O
RCR for the local marine compartment, statistical method	??	[-]	O
RCR for the local fresh-water sediment compartment	0.0193	[-]	O
RCR for the local marine sediment compartment	0.0231	[-]	O
RCR for the local soil compartment	0.0863	[-]	O
RCR for the local soil compartment, statistical method	??	[-]	O
RCR for the sewage treatment plant	9.85E-03	[-]	O
RCR for fish-eating birds and mammals (fresh-water)	1.88E-04	[-]	O
RCR for fish-eating birds and mammals (marine)	2.58E-05	[-]	O
RCR for top predators (marine)	1.2E-05	[-]	O
RCR for worm-eating birds and mammals	4.52E-04	[-]	O
ENVIRONMENT - RISK CHARACTERIZATION			
LOCAL [3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
RCR for the local fresh-water compartment	0.0736	[-]	O
RCR for the local fresh-water compartment, statistical method	??	[-]	O
RCR for the local marine compartment	0.0774	[-]	O
RCR for the local marine compartment, statistical method	??	[-]	O
RCR for the local fresh-water sediment compartment	0.0736	[-]	O
RCR for the local marine sediment compartment	0.0774	[-]	O
RCR for the local soil compartment	0.0886	[-]	O
RCR for the local soil compartment, statistical method	??	[-]	O
RCR for the sewage treatment plant	0.0386	[-]	O
RCR for fish-eating birds and mammals (fresh-water)	1.07E-04	[-]	O
RCR for fish-eating birds and mammals (marine)	1.78E-05	[-]	O
RCR for top predators (marine)	1.03E-05	[-]	O
RCR for worm-eating birds and mammals	4.6E-04	[-]	O
ENVIRONMENT - RISK CHARACTERIZATION			
REGIONAL			
RCR for the regional fresh-water compartment	7.44E-04	[-]	O
RCR for the regional fresh-water compartment, statistical method	??	[-]	O
RCR for the regional marine compartment	4.54E-03	[-]	O
RCR for the regional marine compartment, statistical method	??	[-]	O
RCR for the regional fresh-water sediment compartment	0.0141	[-]	O
RCR for the regional marine sediment compartment	0.141	[-]	O
RCR for the regional soil compartment	0.0838	[-]	O
RCR for the regional soil compartment, statistical method	??	[-]	O

Name	Value	Units	Status
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
Purification factor for surface water	1	[-]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
CONCENTRATIONS IN INTAKE MEDIA [1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
Local concentration in wet fish	7.52E-03	[mg.kg-1]	O
Local concentration in root tissue of plant	3.96	[mg.kg-1]	O
Local concentration in leaves of plant	0.931	[mg.kg-1]	O
Local concentration in grass (wet weight)	0.931	[mg.kg-1]	O
Local concentration in drinking water	4.22	[mg.l-1]	O
Local concentration in meat (wet weight)	2.35E-04	[mg.kg-1]	O
Local concentration in milk (wet weight)	2.35E-03	[mg.kg-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
DOSES IN INTAKE MEDIA [1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
Daily dose through intake of drinking water	0.121	[mg.kg-1.d-1]	O
Daily dose through intake of fish	1.24E-05	[mg.kg-1.d-1]	O
Daily dose through intake of leaf crops	0.016	[mg.kg-1.d-1]	O
Daily dose through intake of root crops	0.0217	[mg.kg-1.d-1]	O
Daily dose through intake of meat	1.01E-06	[mg.kg-1.d-1]	O
Daily dose through intake of milk	1.88E-05	[mg.kg-1.d-1]	O
Daily dose through intake of air	6.62E-09	[mg.kg-1.d-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
FRACTIONS OF TOTAL DOSE [1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
Fraction of total dose through intake of drinking water	0.762	[-]	O
Fraction of total dose through intake of fish	7.81E-05	[-]	O
Fraction of total dose through intake of leaf crops	0.101	[-]	O
Fraction of total dose through intake of root crops	0.137	[-]	O
Fraction of total dose through intake of meat	6.37E-06	[-]	O
Fraction of total dose through intake of milk	1.19E-04	[-]	O
Fraction of total dose through intake of air	4.18E-08	[-]	O
Local total daily intake for humans	0.158	[mg.kg-1.d-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
CONCENTRATIONS IN INTAKE MEDIA [2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
Local concentration in wet fish	0.012	[mg.kg-1]	O
Local concentration in root tissue of plant	0.0356	[mg.kg-1]	O
Local concentration in leaves of plant	0.177	[mg.kg-1]	O
Local concentration in grass (wet weight)	0.177	[mg.kg-1]	O
Local concentration in drinking water	0.0379	[mg.l-1]	O
Local concentration in meat (wet weight)	1.12E-05	[mg.kg-1]	O
Local concentration in milk (wet weight)	1.12E-04	[mg.kg-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
DOSES IN INTAKE MEDIA [2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
Daily dose through intake of drinking water	1.08E-03	[mg.kg-1.d-1]	O
Daily dose through intake of fish	1.98E-05	[mg.kg-1.d-1]	O
Daily dose through intake of leaf crops	3.03E-03	[mg.kg-1.d-1]	O
Daily dose through intake of root crops	1.95E-04	[mg.kg-1.d-1]	O
Daily dose through intake of meat	4.81E-08	[mg.kg-1.d-1]	O
Daily dose through intake of milk	8.96E-07	[mg.kg-1.d-1]	O
Daily dose through intake of air	7.94E-05	[mg.kg-1.d-1]	O

Name	Value	Units	Status
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
FRACTIONS OF TOTAL DOSE [2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
Fraction of total dose through intake of drinking water	0.246	[-]	O
Fraction of total dose through intake of fish	4.49E-03	[-]	O
Fraction of total dose through intake of leaf crops	0.687	[-]	O
Fraction of total dose through intake of root crops	0.0442	[-]	O
Fraction of total dose through intake of meat	1.09E-05	[-]	O
Fraction of total dose through intake of milk	2.03E-04	[-]	O
Fraction of total dose through intake of air	0.018	[-]	O
Local total daily intake for humans	4.41E-03	[mg.kg-1.d-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
CONCENTRATIONS IN INTAKE MEDIA [3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
Local concentration in wet fish	6.68E-03	[mg.kg-1]	O
Local concentration in root tissue of plant	0.0362	[mg.kg-1]	O
Local concentration in leaves of plant	0.239	[mg.kg-1]	O
Local concentration in grass (wet weight)	0.239	[mg.kg-1]	O
Local concentration in drinking water	0.0386	[mg.l-1]	O
Local concentration in meat (wet weight)	1.46E-05	[mg.kg-1]	O
Local concentration in milk (wet weight)	1.46E-04	[mg.kg-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
DOSES IN INTAKE MEDIA [3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
Daily dose through intake of drinking water	1.1E-03	[mg.kg-1.d-1]	O
Daily dose through intake of fish	1.1E-05	[mg.kg-1.d-1]	O
Daily dose through intake of leaf crops	4.1E-03	[mg.kg-1.d-1]	O
Daily dose through intake of root crops	1.98E-04	[mg.kg-1.d-1]	O
Daily dose through intake of meat	6.27E-08	[mg.kg-1.d-1]	O
Daily dose through intake of milk	1.17E-06	[mg.kg-1.d-1]	O
Daily dose through intake of air	1.09E-04	[mg.kg-1.d-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
FRACTIONS OF TOTAL DOSE [3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
Fraction of total dose through intake of drinking water	0.2	[-]	O
Fraction of total dose through intake of fish	1.99E-03	[-]	O
Fraction of total dose through intake of leaf crops	0.743	[-]	O
Fraction of total dose through intake of root crops	0.0359	[-]	O
Fraction of total dose through intake of meat	1.13E-05	[-]	O
Fraction of total dose through intake of milk	2.11E-04	[-]	O
Fraction of total dose through intake of air	0.0197	[-]	O
Local total daily intake for humans	5.52E-03	[mg.kg-1.d-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
REGIONAL SCALE			
CONCENTRATIONS IN INTAKE MEDIA			
Regional concentration in wet fish	4.63E-04	[mg.kg-1]	O
Regional concentration in root tissue of plant	3.08E-04	[mg.kg-1]	O
Regional concentration in leaves of plant	7.48E-05	[mg.kg-1]	O
Regional concentration in grass (wet weight)	7.48E-05	[mg.kg-1]	O
Regional concentration in drinking water	1.23E-04	[mg.l-1]	S
Regional concentration in meat (wet weight)	1.12E-08	[mg.kg-1]	O
Regional concentration in milk (wet weight)	1.12E-07	[mg.kg-1]	O

Name	Value	Units	Status
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
REGIONAL SCALE			
DOSES IN INTAKE MEDIA			
Daily dose through intake of drinking water	3.51E-06	[mg.kg-1.d-1]	O
Daily dose through intake of fish	7.61E-07	[mg.kg-1.d-1]	O
Daily dose through intake of leaf crops	1.28E-06	[mg.kg-1.d-1]	O
Daily dose through intake of root crops	1.69E-06	[mg.kg-1.d-1]	O
Daily dose through intake of meat	4.83E-11	[mg.kg-1.d-1]	O
Daily dose through intake of milk	9.01E-10	[mg.kg-1.d-1]	O
Daily dose through intake of air	1.17E-09	[mg.kg-1.d-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
REGIONAL SCALE			
FRACTIONS OF TOTAL DOSE			
Fraction of total dose through intake of drinking water	0.485	[-]	O
Fraction of total dose through intake of fish	0.105	[-]	O
Fraction of total dose through intake of leaf crops	0.177	[-]	O
Fraction of total dose through intake of root crops	0.233	[-]	O
Fraction of total dose through intake of meat	6.67E-06	[-]	O
Fraction of total dose through intake of milk	1.24E-04	[-]	O
Fraction of total dose through intake of air	1.62E-04	[-]	O
Regional total daily intake for humans	7.25E-06	[mg.kg-1.d-1]	O

Name	Value	Units	Status
HUMAN HEALTH - RISK CHARACTERIZATION			
CURRENT CLASSIFICATION			
Corrosive (C, R34 or R35)	Yes		S
Irritating to skin (Xi, R38)	No		D
Irritating to eyes (Xi, R36)	No		D
Risk of serious damage to eyes (Xi, R41)	No		D
Irritating to respiratory system (Xi, R37)	No		D
May cause sensitisation by inhalation (Xn, R42)	No		D
May cause sensitisation by skin contact (Xi, R43)	No		D
May cause cancer (T, R45)	No		D
May cause cancer by inhalation (T, R49)	No		D
Possible risk of irreversible effects (Xn, R40)	No		D
HUMAN HEALTH - RISK CHARACTERIZATION			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL [1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
MOS, local, inhalatory (repdose)	7.55E+10	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (repdose)	7.55E+10	[-]	O
MOS, local, total exposure (repdose)	6.32E+03	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (repdose)	6.32E+03	[-]	O
MOS, local, inhalatory (fert)	7.55E+10	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (fert)	7.55E+10	[-]	O
MOS, local, total exposure (fert)	6.32E+03	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (fert)	6.32E+03	[-]	O
MOS, local, inhalatory (mattox)	1.13E+10	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (mattox)	1.13E+10	[-]	O
MOS, local, total exposure (mattox)	947	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (mattox)	947	[-]	O
MOS, local, inhalatory (devtox)	1.13E+10	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (devtox)	1.13E+10	[-]	O
MOS, local, total exposure (devtox)	947	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (devtox)	947	[-]	O
HUMAN HEALTH - RISK CHARACTERIZATION			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL [2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
MOS, local, inhalatory (repdose)	6.29E+06	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (repdose)	6.29E+06	[-]	O
MOS, local, total exposure (repdose)	2.27E+05	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (repdose)	2.27E+05	[-]	O
MOS, local, inhalatory (fert)	6.29E+06	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (fert)	6.29E+06	[-]	O
MOS, local, total exposure (fert)	2.27E+05	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (fert)	2.27E+05	[-]	O
MOS, local, inhalatory (mattox)	9.44E+05	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (mattox)	9.44E+05	[-]	O
MOS, local, total exposure (mattox)	3.4E+04	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (mattox)	3.4E+04	[-]	O
MOS, local, inhalatory (devtox)	9.44E+05	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (devtox)	9.44E+05	[-]	O
MOS, local, total exposure (devtox)	3.4E+04	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (devtox)	3.4E+04	[-]	O

Name	Value	Units	Status
HUMAN HEALTH - RISK CHARACTERIZATION			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL [3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
MOS, local, inhalatory (repdose)	4.6E+06	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (repdose)	4.6E+06	[-]	O
MOS, local, total exposure (repdose)	1.81E+05	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (repdose)	1.81E+05	[-]	O
MOS, local, inhalatory (fert)	4.6E+06	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (fert)	4.6E+06	[-]	O
MOS, local, total exposure (fert)	1.81E+05	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (fert)	1.81E+05	[-]	O
MOS, local, inhalatory (mattox)	6.89E+05	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (mattox)	6.89E+05	[-]	O
MOS, local, total exposure (mattox)	2.72E+04	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (mattox)	2.72E+04	[-]	O
MOS, local, inhalatory (devtox)	6.89E+05	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (devtox)	6.89E+05	[-]	O
MOS, local, total exposure (devtox)	2.72E+04	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (devtox)	2.72E+04	[-]	O
HUMAN HEALTH - RISK CHARACTERIZATION			
HUMANS EXPOSED VIA THE ENVIRONMENT			
REGIONAL			
MOS, regional, inhalatory (repdose)	4.27E+11	[-]	O
Ratio MOS/Ref-MOS, regional, inhalatory (repdose)	4.27E+11	[-]	O
MOS, regional, total exposure (repdose)	1.38E+08	[-]	O
Ratio MOS/Ref-MOS, regional, total exposure (repdose)	1.38E+08	[-]	O
MOS, regional, inhalatory (fert)	4.27E+11	[-]	O
Ratio MOS/Ref-MOS, regional, inhalatory (fert)	4.27E+11	[-]	O
MOS, regional, total exposure (fert)	1.38E+08	[-]	O
Ratio MOS/Ref-MOS, regional, total exposure (fert)	1.38E+08	[-]	O
MOS, regional, inhalatory (mattox)	6.4E+10	[-]	O
Ratio MOS/Ref-MOS, regional, inhalatory (mattox)	6.4E+10	[-]	O
MOS, regional, total exposure (mattox)	2.07E+07	[-]	O
Ratio MOS/Ref-MOS, regional, total exposure (mattox)	2.07E+07	[-]	O
MOS, regional, inhalatory (devtox)	6.4E+10	[-]	O
Ratio MOS/Ref-MOS, regional, inhalatory (devtox)	6.4E+10	[-]	O
MOS, regional, total exposure (devtox)	2.07E+07	[-]	O
Ratio MOS/Ref-MOS, regional, total exposure (devtox)	2.07E+07	[-]	O

Printed on	15-12-2017 17:03:36
Study	TFA 2100 Plateau, low EC50
Substance	Trifluoroacetic acid
Defaults	Standard Euses 2.1
Assessment types	1A, 1B, 2, 3A, 3B
Base set complete	No
Explanation status column	O = Output; D = Default; S = Set; I = Imported

Name	Value	Units	Status
IDENTIFICATION OF THE SUBSTANCE			
General name	Trifluoroacetic acid		S
CAS-No	76-05-1		S
EC-notification no.	200-929-3		S
EINECS no.	200-929-3		S
Molecular weight	114.02	[g.mol-1]	S

Printed on	15-12-2017 17:03:36
Study	Trifluoroacetic acid
Substance	TFA 2100 Plateau, low EC50
Defaults	Standard Euses 2.1
Assessment types	1A, 1B, 2, 3A, 3B
Base set complete	No

Name	Value	Units	Status
PHYSICO-CHEMICAL PROPERTIES			
Melting point	-15.2	[oC]	S
Boiling point	71.78	[oC]	S
Vapour pressure at test temperature	1.58E+04	[Pa]	S
Vapour pressure at 25 [oC]	1.58E+04	[Pa]	O
Water solubility at test temperature	1E+05	[mg.l-1]	S
Water solubility at 25 [oC]	1E+05	[mg.l-1]	O
Octanol-water partition coefficient	-0.2	[log10]	S
Henry's law constant at 25 [oC]	7.13E-03	[Pa.m3.mol-1]	S

Name	Value	Units	Status
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
Tonnage of substance in Europe	1.2E+05	[tonnes.yr-1]	O
Regional production volume of substance	1E+05	[tonnes.yr-1]	O
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
[1 "CHEMICAL PRODUCTION", IC=3/UC=29]			
Industry category	3 Chemical industry: chemicals used in synthesis		S
Use category	29 Heat transferring agents		S
Fraction of tonnage for application	100	[%]	O
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
[PRODUCTION]			
Use specific emission scenario	No		D
Emission tables	A1.1 (general table), B1.6 (general table)		S
Emission scenario	no special scenario selected/available		S
Main category production	Ib Intermed. stored on-site/continuous prod.		S
Fraction of tonnage released to air	0.95	[-]	S
Fraction of tonnage released to wastewater	1.5E-03	[-]	S
Fraction of tonnage released to surface water	0.015	[-]	S
Fraction of tonnage released to industrial soil	0.015	[-]	S
Fraction of tonnage released to agricultural soil	0.015	[-]	S
Fraction of the main local source	0.1	[-]	S
Number of emission days per year	300	[-]	O
Local emission to air during episode	1.4815E+04	[kg.d-1]	S
Local emission to wastewater during episode	150	[kg.d-1]	S
Intermittent release	Yes		S
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
[2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29]			
Industry category	5 Personal / domestic use		S
Use category	29 Heat transferring agents		S
Fraction of tonnage for application	65	[%]	S
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
[PRIVATE USE]			
Use specific emission scenario	No		D
Emission tables	A4.1 (specific uses), B4.1 (general table)		S
Emission scenario	no special scenario selected/available		S
Fraction of tonnage released to air	0.95	[-]	S
Fraction of tonnage released to wastewater	5E-03	[-]	S
Fraction of tonnage released to surface water	0.015	[-]	S
Fraction of tonnage released to industrial soil	0.015	[-]	S
Fraction of tonnage released to agricultural soil	0.015	[-]	S
Fraction of the main local source	0.65	[-]	S
Number of emission days per year	365	[-]	O
Local emission to air during episode	2	[kg.d-1]	S
Local emission to wastewater during episode	226	[kg.d-1]	O
Intermittent release	No		D
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
[3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29]			
Industry category	6 Public domain		S
Use category	29 Heat transferring agents		S
Fraction of tonnage for application	0.35	[-]	S

Printed on	15-12-2017 17:03:36
Study	Trifluoroacetic acid
Substance	TFA 2100 Plateau, low EC50
Defaults	Standard Euses 2.1
Assessment types	1A, 1B, 2, 3A, 3B
Base set complete	No

Name	Value	Units	Status
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
[INDUSTRIAL USE]			
Use specific emission scenario	No		D
Emission tables	A3.5 (specific uses), B3.3 (specific uses)		S
Emission scenario	no special scenario selected/available		S
Fraction of tonnage released to air	0.95	[-]	S
Fraction of tonnage released to wastewater	5E-03	[-]	S
Fraction of tonnage released to surface water	0.015	[-]	S
Fraction of tonnage released to industrial soil	0.015	[-]	S
Fraction of tonnage released to agricultural soil	0.015	[-]	S
Fraction of the main local source	0.35	[-]	S
Number of emission days per year	50	[-]	O
Local emission to air during episode	15	[kg.d-1]	S
Local emission to wastewater during episode	478	[kg.d-1]	O
Intermittent release	No		D
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
TOTAL REGIONAL EMISSIONS TO COMPARTMENTS			
Total regional emission to air	1.07116E+05	[kg.d-1]	S
Total regional emission to wastewater	1.0711E+04	[kg.d-1]	S
Total regional emission to surface water	5.3558E+04	[kg.d-1]	S
Total regional emission to industrial soil	2.1423E+04	[kg.d-1]	S
Total regional emission to agricultural soil	2.1423E+04	[kg.d-1]	S
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
TOTAL CONTINENTAL EMISSIONS TO COMPARTMENTS			
Total continental emission to air	3.21349E+05	[kg.d-1]	S
Total continental emission to wastewater	3.2134E+04	[kg.d-1]	S
Total continental emission to surface water	1.60674E+05	[kg.d-1]	S
Total continental emission to industrial soil	6.4269E+04	[kg.d-1]	S
Total continental emission to agricultural soil	6.4269E+04	[kg.d-1]	S
ENVIRONMENT-EXPOSURE			
PARTITION COEFFICIENTS			
Organic carbon-water partition coefficient	1	[l.kg-1]	S
ENVIRONMENT-EXPOSURE			
DEGRADATION AND TRANSFORMATION			
Characterization of biodegradability	Not biodegradable		S
Degradation calculation method in STP	First order, standard OECD/EU tests		D
Rate constant for biodegradation in STP	0	[d-1]	O
Rate constant for biodegradation in surface water	0	[d-1] (12[oC])	O
Rate constant for biodegradation in bulk soil	6.93E-07	[d-1] (12[oC])	O
Rate constant for biodegradation in aerated sediment	6.93E-07	[d-1] (12[oC])	O
Rate constant for hydrolysis in surface water	6.93E-07	[d-1] (12[oC])	O
Rate constant for photolysis in surface water	6.93E-07	[d-1]	O
ENVIRONMENT-EXPOSURE			
SEWAGE TREATMENT			
LOCAL STP [1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
OUTPUT			
Fraction of emission directed to air by STP	6.83E-03	[%]	O
Fraction of emission directed to water by STP	100	[%]	O
Fraction of emission directed to sludge by STP	0.0125	[%]	O
Fraction of the emission degraded in STP	0	[%]	O
Concentration in untreated wastewater	7.5E+04	[ug.l-1]	O
Concentration of chemical (total) in the STP-effluent	75	[mg.l-1]	O
Concentration in effluent exceeds solubility	No		O
Concentration in dry sewage sludge	23.8	[mg.kg-1]	O
PEC for micro-organisms in the STP	75	[mg.l-1]	O

Printed on	15-12-2017 17:03:36
Study	Trifluoroacetic acid
Substance	TFA 2100 Plateau, low EC50
Defaults	Standard Euses 2.1
Assessment types	1A, 1B, 2, 3A, 3B
Base set complete	No

Name	Value	Units	Status
ENVIRONMENT-EXPOSURE			
SEWAGE TREATMENT			
LOCAL STP [2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
OUTPUT			
Fraction of emission directed to air by STP	6.83E-03	[%]	O
Fraction of emission directed to water by STP	100	[%]	O
Fraction of emission directed to sludge by STP	0.0125	[%]	O
Fraction of the emission degraded in STP	0	[%]	O
Concentration in untreated wastewater	113	[mg.l-1]	O
Concentration of chemical (total) in the STP-effluent	113	[mg.l-1]	O
Concentration in effluent exceeds solubility	No		O
Concentration in dry sewage sludge	35.8	[mg.kg-1]	O
PEC for micro-organisms in the STP	113	[mg.l-1]	O
ENVIRONMENT-EXPOSURE			
SEWAGE TREATMENT			
LOCAL STP [3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
OUTPUT			
Fraction of emission directed to air by STP	6.83E-03	[%]	O
Fraction of emission directed to water by STP	100	[%]	O
Fraction of emission directed to sludge by STP	0.0125	[%]	O
Fraction of the emission degraded in STP	0	[%]	O
Concentration in untreated wastewater	239	[mg.l-1]	O
Concentration of chemical (total) in the STP-effluent	239	[mg.l-1]	O
Concentration in effluent exceeds solubility	No		O
Concentration in dry sewage sludge	75.7	[mg.kg-1]	O
PEC for micro-organisms in the STP	239	[mg.l-1]	O
ENVIRONMENT-EXPOSURE			
SEWAGE TREATMENT			
REGIONAL STP			
Fraction of emission directed to air	10	[%]	S
Fraction of emission directed to water	90	[%]	S
ENVIRONMENT-EXPOSURE			
SEWAGE TREATMENT			
CONTINENTAL STP			
Fraction of emission directed to air	10	[%]	S
Fraction of emission directed to water	90	[%]	S
Fraction of the emission degraded	0	[%]	S
ENVIRONMENT-EXPOSURE			
DISTRIBUTION			
LOCAL SCALE			
DEFAULT VALUES FOR LOCAL SCALE			
Calculate dilution from river flow rate	No		S
ENVIRONMENT-EXPOSURE			
DISTRIBUTION			
LOCAL SCALE			
[1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
Concentration in air during emission episode	2.9E-08	[mg.m-3]	S
Annual average concentration in air, 100 m from point source	2.38E-08	[mg.m-3]	O
Concentration in surface water during emission episode (dissolved)	7.5	[mg.l-1]	O
Annual average concentration in surface water (dissolved)	6.16	[mg.l-1]	O
Local PEC in surface water during emission episode (dissolved)	7.5	[mg.l-1]	O
Annual average local PEC in surface water (dissolved)	6.16	[mg.l-1]	O
Local PEC in fresh-water sediment during emission episode	6.03	[mg.kgwwt-1]	O
Concentration in seawater during emission episode (dissolved)	0.75	[mg.l-1]	O
Annual average concentration in seawater (dissolved)	0.616	[mg.l-1]	O
Local PEC in seawater during emission episode (dissolved)	0.75	[mg.l-1]	O
Annual average local PEC in seawater (dissolved)	0.617	[mg.l-1]	O
Local PEC in marine sediment during emission episode	0.603	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 30 days	1.45	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 180 days	1.43	[mg.kgwwt-1]	O
Local PEC in grassland (total) averaged over 180 days	1.42	[mg.kgwwt-1]	O
Local PEC in groundwater under agricultural soil	10.6	[mg.l-1]	O

Name	Value	Units	Status
ENVIRONMENT-EXPOSURE			
DISTRIBUTION			
LOCAL SCALE			
[2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
Concentration in air during emission episode	5.56E-04	[mg.m-3]	O
Annual average concentration in air, 100 m from point source	5.56E-04	[mg.m-3]	O
Concentration in surface water during emission episode (dissolved)	11.3	[mg.l-1]	O
Annual average concentration in surface water (dissolved)	11.3	[mg.l-1]	O
Local PEC in surface water during emission episode (dissolved)	11.3	[mg.l-1]	O
Annual average local PEC in surface water (dissolved)	11.3	[mg.l-1]	O
Local PEC in fresh-water sediment during emission episode	9.1	[mg.kgwwt-1]	O
Concentration in seawater during emission episode (dissolved)	1.13	[mg.l-1]	O
Annual average concentration in seawater (dissolved)	1.13	[mg.l-1]	O
Local PEC in seawater during emission episode (dissolved)	1.13	[mg.l-1]	O
Annual average local PEC in seawater (dissolved)	1.13	[mg.l-1]	O
Local PEC in marine sediment during emission episode	0.91	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 30 days	0.0495	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 180 days	0.0262	[mg.kgwwt-1]	O
Local PEC in grassland (total) averaged over 180 days	9.81E-03	[mg.kgwwt-1]	O
Local PEC in groundwater under agricultural soil	0.194	[mg.l-1]	O
ENVIRONMENT-EXPOSURE			
DISTRIBUTION			
LOCAL SCALE			
[3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
Concentration in air during emission episode	4.17E-03	[mg.m-3]	O
Annual average concentration in air, 100 m from point source	5.71E-04	[mg.m-3]	O
Concentration in surface water during emission episode (dissolved)	23.9	[mg.l-1]	O
Annual average concentration in surface water (dissolved)	3.27	[mg.l-1]	O
Local PEC in surface water during emission episode (dissolved)	23.9	[mg.l-1]	O
Annual average local PEC in surface water (dissolved)	3.27	[mg.l-1]	O
Local PEC in fresh-water sediment during emission episode	19.2	[mg.kgwwt-1]	O
Concentration in seawater during emission episode (dissolved)	2.39	[mg.l-1]	O
Annual average concentration in seawater (dissolved)	0.327	[mg.l-1]	O
Local PEC in seawater during emission episode (dissolved)	2.39	[mg.l-1]	O
Annual average local PEC in seawater (dissolved)	0.327	[mg.l-1]	O
Local PEC in marine sediment during emission episode	1.92	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 30 days	0.0988	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 180 days	0.0495	[mg.kgwwt-1]	O
Local PEC in grassland (total) averaged over 180 days	0.0149	[mg.kgwwt-1]	O
Local PEC in groundwater under agricultural soil	0.366	[mg.l-1]	O
ENVIRONMENT-EXPOSURE			
DISTRIBUTION			
REGIONAL AND CONTINENTAL SCALE			
CONTINENTAL			
Continental PEC in surface water (dissolved)	8.17E-03	[mg.l-1]	O
Continental PEC in seawater (dissolved)	2.2E-03	[mg.l-1]	O
Continental PEC in air (total)	8.38E-03	[mg.m-3]	O
Continental PEC in agricultural soil (total)	3.41E-03	[mg.kgwwt-1]	O
Continental PEC in pore water of agricultural soils	0.0251	[mg.l-1]	O
Continental PEC in natural soil (total)	5.21E-04	[mg.kgwwt-1]	O
Continental PEC in industrial soil (total)	0.0179	[mg.kgwwt-1]	O
Continental PEC in sediment (total)	5.72E-03	[mg.kgwwt-1]	O
Continental PEC in seawater sediment (total)	1.56E-03	[mg.kgwwt-1]	O

Name	Value	Units	Status
ENVIRONMENT-EXPOSURE			
DISTRIBUTION			
REGIONAL AND CONTINENTAL SCALE			
REGIONAL			
Regional PEC in surface water (dissolved)	3.28E-04	[mg.l-1]	S
Regional PEC in seawater (dissolved)	2E-04	[mg.l-1]	S
Regional PEC in air (total)	4.1E-09	[mg.m-3]	S
Regional PEC in agricultural soil (total)	5E-03	[mg.kgwwt-1]	S
Regional PEC in pore water of agricultural soils	3.28E-04	[mg.l-1]	S
Regional PEC in natural soil (total)	5E-03	[mg.kgwwt-1]	S
Regional PEC in industrial soil (total)	5E-03	[mg.kgwwt-1]	S
Regional PEC in sediment (total)	5E-03	[mg.kgwwt-1]	S
Regional PEC in seawater sediment (total)	5E-03	[mg.kgwwt-1]	S
ENVIRONMENT-EXPOSURE			
BIOCONCENTRATION			
Bioconcentration factor for earthworms	0.848	[l.kgwwt-1]	O
Bioconcentration factor for fish	1.41	[l.kgwwt-1]	O
ENVIRONMENT-EXPOSURE			
SECONDARY POISONING [1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
Concentration in fish for secondary poisoning (freshwater)	4.35	[mg.kgwwt-1]	O
Concentration in fish for secondary poisoning (marine)	0.436	[mg.kgwwt-1]	O
Concentration in fish-eating marine top-predators	0.0873	[mg.kgwwt-1]	O
Concentration in earthworms from agricultural soil	4.11	[mg.kg-1]	O
ENVIRONMENT-EXPOSURE			
SECONDARY POISONING [2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
Concentration in fish for secondary poisoning (freshwater)	7.99	[mg.kgwwt-1]	O
Concentration in fish for secondary poisoning (marine)	0.799	[mg.kgwwt-1]	O
Concentration in fish-eating marine top-predators	0.16	[mg.kgwwt-1]	O
Concentration in earthworms from agricultural soil	0.0754	[mg.kg-1]	O
ENVIRONMENT-EXPOSURE			
SECONDARY POISONING [3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
Concentration in fish for secondary poisoning (freshwater)	2.31	[mg.kgwwt-1]	O
Concentration in fish for secondary poisoning (marine)	0.231	[mg.kgwwt-1]	O
Concentration in fish-eating marine top-predators	0.0465	[mg.kgwwt-1]	O
Concentration in earthworms from agricultural soil	0.142	[mg.kg-1]	O

Name	Value	Units	Status
ENVIRONMENT - EFFECTS			
MICRO-ORGANISMS			
Test system	Respiration inhibition, EU Annex V C.11, OECD 209		D
EC50 for micro-organisms in a STP	832	[mg.l-1]	S
EC10 for micro-organisms in a STP	832	[mg.l-1]	S
NOEC for micro-organisms in a STP	832	[mg.l-1]	S
PNEC for micro-organisms in a STP	8.32	[mg.l-1]	O
Assessment factor applied in extrapolation to PNEC micro	10	[-]	S
ENVIRONMENT - EFFECTS			
FRESH_WATER ORGANISMS			
LC50 for fish	1.2E+03	[mg.l-1]	S
L(E)C50 for Daphnia	1.2E+03	[mg.l-1]	S
EC50 for algae	0.62	[mg.l-1]	S
LC50 for additional taxonomic group	??	[mg.l-1]	D
NOEC for fish	??	[mg.l-1]	D
NOEC for Daphnia	??	[mg.l-1]	D
NOEC for algae	??	[mg.l-1]	D
NOEC for additional taxonomic group	??	[mg.l-1]	D
PNEC for aquatic organisms	6.2E-04	[mg.l-1]	O
PNEC for aquatic organisms, intermittent releases	6.2E-03	[mg.l-1]	O
ENVIRONMENT - EFFECTS			
MARINE ORGANISMS			
LC50 for fish (marine)	??	[mg.l-1]	D
L(E)C50 for crustaceans (marine)	??	[mg.l-1]	D
EC50 for algae (marine)	97	[mg.l-1]	S
LC50 for additional taxonomic group (marine)	??	[mg.l-1]	D
NOEC for fish (marine)	??	[mg.l-1]	D
NOEC for crustaceans (marine)	??	[mg.l-1]	D
NOEC for algae (marine)	??	[mg.l-1]	D
NOEC for additional taxonomic group (marine)	??	[mg.l-1]	D
PNEC for marine organisms	6.2E-05	[mg.l-1]	O
ENVIRONMENT - EFFECTS			
FRESH-WATER SEDIMENT ORGANISMS			
LC50 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
PNEC for fresh-water sediment, normalised to 5% o.c. (regional)	4.99E-04	[mg.kgwwt-1]	O
ENVIRONMENT - EFFECTS			
MARINE SEDIMENT ORGANISMS			
LC50 for marine sediment organism	??	[mg.kgwwt-1]	D
EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D
PNEC for marine sediment, normalised to 5% o.c. (regional)	4.99E-05	[mg.kgwwt-1]	O

Name	Value	Units	Status
ENVIRONMENT - EFFECTS			
TERRESTRIAL ORGANISMS			
LC50 for plants	250	[mg.kgdwt-1]	S
LC50 for earthworms	??	[mg.kgwwt-1]	D
EC50 for microorganisms	??	[mg.kgwwt-1]	D
LC50 for other terrestrial species	??	[mg.kgwwt-1]	D
NOEC for plants	??	[mg.kgwwt-1]	D
NOEC for earthworms	??	[mg.kgwwt-1]	D
NOEC for microorganisms	??	[mg.kgwwt-1]	D
NOEC for additional taxonomic group	??	[mg.kgwwt-1]	D
NOEC for additional taxonomic group	??	[mg.kgwwt-1]	D
PNEC for terrestrial organisms	8.39E-05	[mg.kgwwt-1]	O
Equilibrium partitioning used for PNEC in soil?	Yes		O
ENVIRONMENT - EFFECTS			
BIRDS AND MAMMALS			
Oral NOAEL (repdose)	1E+03	[mg.kg-1.d-1]	S
NOEC via food (repdose)	1E+04	[mg.kg-1]	O
Inhalatory NOAEL (repdose)	1.75E+03	[mg.m-3]	O
Dermal NOAEL (repdose)	1E+03	[mg.kg-1.d-1]	O
Oral NOAEL (fert)	1E+03	[mg.kg-1.d-1]	S
NOEC via food (fert)	1E+04	[mg.kg-1]	O
Inhalatory NOAEL (fert)	1.75E+03	[mg.m-3]	O
Dermal NOAEL (fert)	1E+03	[mg.kg-1.d-1]	O
Oral NOAEL (mattox)	150	[mg.kg-1.d-1]	S
NOEC via food (mattox)	1.5E+03	[mg.kg-1]	O
Inhalatory NOAEL (mattox)	262	[mg.m-3]	O
Dermal NOAEL (mattox)	150	[mg.kg-1.d-1]	O
Oral NOAEL (devtox)	150	[mg.kg-1.d-1]	S
NOEC via food (devtox)	1.5E+03	[mg.kg-1]	O
Inhalatory NOAEL (devtox)	262	[mg.m-3]	O
Dermal NOAEL (devtox)	150	[mg.kg-1.d-1]	O
Duration of (sub-)chronic oral test	28 days		D
NOEC via food for secondary poisoning	1E+04	[mg.kg-1]	O
PNEC for secondary poisoning of birds and mammals	33.3	[mg.kg-1]	O

Name	Value	Units	Status
ENVIRONMENT - RISK CHARACTERIZATION			
LOCAL [1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
RCR for the local fresh-water compartment	1.21E+03	[-]	O
RCR for the local fresh-water compartment, statistical method	??	[-]	O
RCR for the local marine compartment	1.21E+04	[-]	O
RCR for the local marine compartment, statistical method	??	[-]	O
RCR for the local fresh-water sediment compartment	1.21E+04	[-]	O
RCR for the local marine sediment compartment	1.21E+04	[-]	O
RCR for the local soil compartment	1.73E+04	[-]	O
RCR for the local soil compartment, statistical method	??	[-]	O
RCR for the sewage treatment plant	9.01	[-]	O
RCR for fish-eating birds and mammals (fresh-water)	0.131	[-]	O
RCR for fish-eating birds and mammals (marine)	0.0131	[-]	O
RCR for top predators (marine)	2.62E-03	[-]	O
RCR for worm-eating birds and mammals	0.123	[-]	O
ENVIRONMENT - RISK CHARACTERIZATION			
LOCAL [2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
RCR for the local fresh-water compartment	1.82E+04	[-]	O
RCR for the local fresh-water compartment, statistical method	??	[-]	O
RCR for the local marine compartment	1.82E+04	[-]	O
RCR for the local marine compartment, statistical method	??	[-]	O
RCR for the local fresh-water sediment compartment	1.82E+04	[-]	O
RCR for the local marine sediment compartment	1.82E+04	[-]	O
RCR for the local soil compartment	590	[-]	O
RCR for the local soil compartment, statistical method	??	[-]	O
RCR for the sewage treatment plant	13.6	[-]	O
RCR for fish-eating birds and mammals (fresh-water)	0.24	[-]	O
RCR for fish-eating birds and mammals (marine)	0.024	[-]	O
RCR for top predators (marine)	4.8E-03	[-]	O
RCR for worm-eating birds and mammals	2.26E-03	[-]	O
ENVIRONMENT - RISK CHARACTERIZATION			
LOCAL [3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
RCR for the local fresh-water compartment	3.85E+04	[-]	O
RCR for the local fresh-water compartment, statistical method	??	[-]	O
RCR for the local marine compartment	3.85E+04	[-]	O
RCR for the local marine compartment, statistical method	??	[-]	O
RCR for the local fresh-water sediment compartment	3.85E+04	[-]	O
RCR for the local marine sediment compartment	3.85E+04	[-]	O
RCR for the local soil compartment	1.18E+03	[-]	O
RCR for the local soil compartment, statistical method	??	[-]	O
RCR for the sewage treatment plant	28.7	[-]	O
RCR for fish-eating birds and mammals (fresh-water)	0.0693	[-]	O
RCR for fish-eating birds and mammals (marine)	6.94E-03	[-]	O
RCR for top predators (marine)	1.4E-03	[-]	O
RCR for worm-eating birds and mammals	4.27E-03	[-]	O
ENVIRONMENT - RISK CHARACTERIZATION			
REGIONAL			
RCR for the regional fresh-water compartment	0.529	[-]	O
RCR for the regional fresh-water compartment, statistical method	??	[-]	O
RCR for the regional marine compartment	3.23	[-]	O
RCR for the regional marine compartment, statistical method	??	[-]	O
RCR for the regional fresh-water sediment compartment	10	[-]	O
RCR for the regional marine sediment compartment	100	[-]	O
RCR for the regional soil compartment	59.6	[-]	O
RCR for the regional soil compartment, statistical method	??	[-]	O

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Study	Trifluoroacetic acid
Substance	TFA 2100 Plateau, low EC50
Defaults	Standard Euses 2.1
Assessment types	1A, 1B, 2, 3A, 3B
Base set complete	No

Name	Value	Units	Status
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
Purification factor for surface water	1	[-]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
CONCENTRATIONS IN INTAKE MEDIA [1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
Local concentration in wet fish	8.71	[mg.kg-1]	O
Local concentration in root tissue of plant	9.94	[mg.kg-1]	O
Local concentration in leaves of plant	2.34	[mg.kg-1]	O
Local concentration in grass (wet weight)	2.32	[mg.kg-1]	O
Local concentration in drinking water	10.6	[mg.l-1]	O
Local concentration in meat (wet weight)	5.88E-04	[mg.kg-1]	O
Local concentration in milk (wet weight)	5.88E-03	[mg.kg-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
DOSES IN INTAKE MEDIA [1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
Daily dose through intake of drinking water	0.303	[mg.kg-1.d-1]	O
Daily dose through intake of fish	0.0143	[mg.kg-1.d-1]	O
Daily dose through intake of leaf crops	0.0401	[mg.kg-1.d-1]	O
Daily dose through intake of root crops	0.0545	[mg.kg-1.d-1]	O
Daily dose through intake of meat	2.53E-06	[mg.kg-1.d-1]	O
Daily dose through intake of milk	4.72E-05	[mg.kg-1.d-1]	O
Daily dose through intake of air	7.98E-09	[mg.kg-1.d-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
FRACTIONS OF TOTAL DOSE [1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
Fraction of total dose through intake of drinking water	0.735	[-]	O
Fraction of total dose through intake of fish	0.0347	[-]	O
Fraction of total dose through intake of leaf crops	0.0973	[-]	O
Fraction of total dose through intake of root crops	0.132	[-]	O
Fraction of total dose through intake of meat	6.14E-06	[-]	O
Fraction of total dose through intake of milk	1.14E-04	[-]	O
Fraction of total dose through intake of air	1.94E-08	[-]	O
Local total daily intake for humans	0.412	[mg.kg-1.d-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
CONCENTRATIONS IN INTAKE MEDIA [2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
Local concentration in wet fish	16	[mg.kg-1]	O
Local concentration in root tissue of plant	0.182	[mg.kg-1]	O
Local concentration in leaves of plant	0.38	[mg.kg-1]	O
Local concentration in grass (wet weight)	0.353	[mg.kg-1]	O
Local concentration in drinking water	11.3	[mg.l-1]	O
Local concentration in meat (wet weight)	5.13E-04	[mg.kg-1]	O
Local concentration in milk (wet weight)	5.13E-03	[mg.kg-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
DOSES IN INTAKE MEDIA [2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
Daily dose through intake of drinking water	0.323	[mg.kg-1.d-1]	O
Daily dose through intake of fish	0.0262	[mg.kg-1.d-1]	O
Daily dose through intake of leaf crops	6.51E-03	[mg.kg-1.d-1]	O
Daily dose through intake of root crops	9.96E-04	[mg.kg-1.d-1]	O
Daily dose through intake of meat	2.21E-06	[mg.kg-1.d-1]	O
Daily dose through intake of milk	4.11E-05	[mg.kg-1.d-1]	O
Daily dose through intake of air	1.59E-04	[mg.kg-1.d-1]	O

Name	Value	Units	Status
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
FRACTIONS OF TOTAL DOSE [2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
Fraction of total dose through intake of drinking water	0.905	[-]	O
Fraction of total dose through intake of fish	0.0735	[-]	O
Fraction of total dose through intake of leaf crops	0.0182	[-]	O
Fraction of total dose through intake of root crops	2.79E-03	[-]	O
Fraction of total dose through intake of meat	6.18E-06	[-]	O
Fraction of total dose through intake of milk	1.15E-04	[-]	O
Fraction of total dose through intake of air	4.45E-04	[-]	O
Local total daily intake for humans	0.357	[mg.kg-1.d-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
CONCENTRATIONS IN INTAKE MEDIA [3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
Local concentration in wet fish	4.62	[mg.kg-1]	O
Local concentration in root tissue of plant	0.343	[mg.kg-1]	O
Local concentration in leaves of plant	0.427	[mg.kg-1]	O
Local concentration in grass (wet weight)	0.371	[mg.kg-1]	O
Local concentration in drinking water	3.27	[mg.l-1]	O
Local concentration in meat (wet weight)	1.63E-04	[mg.kg-1]	O
Local concentration in milk (wet weight)	1.63E-03	[mg.kg-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
DOSES IN INTAKE MEDIA [3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
Daily dose through intake of drinking water	0.0935	[mg.kg-1.d-1]	O
Daily dose through intake of fish	7.59E-03	[mg.kg-1.d-1]	O
Daily dose through intake of leaf crops	7.32E-03	[mg.kg-1.d-1]	O
Daily dose through intake of root crops	1.88E-03	[mg.kg-1.d-1]	O
Daily dose through intake of meat	7.01E-07	[mg.kg-1.d-1]	O
Daily dose through intake of milk	1.31E-05	[mg.kg-1.d-1]	O
Daily dose through intake of air	1.63E-04	[mg.kg-1.d-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
FRACTIONS OF TOTAL DOSE [3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
Fraction of total dose through intake of drinking water	0.846	[-]	O
Fraction of total dose through intake of fish	0.0687	[-]	O
Fraction of total dose through intake of leaf crops	0.0663	[-]	O
Fraction of total dose through intake of root crops	0.0171	[-]	O
Fraction of total dose through intake of meat	6.34E-06	[-]	O
Fraction of total dose through intake of milk	1.18E-04	[-]	O
Fraction of total dose through intake of air	1.48E-03	[-]	O
Local total daily intake for humans	0.11	[mg.kg-1.d-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
REGIONAL SCALE			
CONCENTRATIONS IN INTAKE MEDIA			
Regional concentration in wet fish	4.63E-04	[mg.kg-1]	O
Regional concentration in root tissue of plant	3.08E-04	[mg.kg-1]	O
Regional concentration in leaves of plant	7.48E-05	[mg.kg-1]	O
Regional concentration in grass (wet weight)	7.48E-05	[mg.kg-1]	O
Regional concentration in drinking water	1.23E-04	[mg.l-1]	S
Regional concentration in meat (wet weight)	1.12E-08	[mg.kg-1]	O
Regional concentration in milk (wet weight)	1.12E-07	[mg.kg-1]	O

Name	Value	Units	Status
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
REGIONAL SCALE			
DOSES IN INTAKE MEDIA			
Daily dose through intake of drinking water	3.51E-06	[mg.kg-1.d-1]	O
Daily dose through intake of fish	7.61E-07	[mg.kg-1.d-1]	O
Daily dose through intake of leaf crops	1.28E-06	[mg.kg-1.d-1]	O
Daily dose through intake of root crops	1.69E-06	[mg.kg-1.d-1]	O
Daily dose through intake of meat	4.83E-11	[mg.kg-1.d-1]	O
Daily dose through intake of milk	9.01E-10	[mg.kg-1.d-1]	O
Daily dose through intake of air	1.17E-09	[mg.kg-1.d-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
REGIONAL SCALE			
FRACTIONS OF TOTAL DOSE			
Fraction of total dose through intake of drinking water	0.485	[-]	O
Fraction of total dose through intake of fish	0.105	[-]	O
Fraction of total dose through intake of leaf crops	0.177	[-]	O
Fraction of total dose through intake of root crops	0.233	[-]	O
Fraction of total dose through intake of meat	6.67E-06	[-]	O
Fraction of total dose through intake of milk	1.24E-04	[-]	O
Fraction of total dose through intake of air	1.62E-04	[-]	O
Regional total daily intake for humans	7.25E-06	[mg.kg-1.d-1]	O

Name	Value	Units	Status
HUMAN HEALTH - RISK CHARACTERIZATION			
CURRENT CLASSIFICATION			
Corrosive (C, R34 or R35)	Yes		S
Irritating to skin (Xi, R38)	No		D
Irritating to eyes (Xi, R36)	No		D
Risk of serious damage to eyes (Xi, R41)	No		D
Irritating to respiratory system (Xi, R37)	No		D
May cause sensitisation by inhalation (Xn, R42)	No		D
May cause sensitisation by skin contact (Xi, R43)	No		D
May cause cancer (T, R45)	No		D
May cause cancer by inhalation (T, R49)	No		D
Possible risk of irreversible effects (Xn, R40)	No		D
HUMAN HEALTH - RISK CHARACTERIZATION			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL [1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
MOS, local, inhalatory (repdose)	6.26E+10	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (repdose)	6.26E+10	[-]	O
MOS, local, total exposure (repdose)	2.43E+03	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (repdose)	2.43E+03	[-]	O
MOS, local, inhalatory (fert)	6.26E+10	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (fert)	6.26E+10	[-]	O
MOS, local, total exposure (fert)	2.43E+03	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (fert)	2.43E+03	[-]	O
MOS, local, inhalatory (mattox)	9.4E+09	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (mattox)	9.4E+09	[-]	O
MOS, local, total exposure (mattox)	364	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (mattox)	364	[-]	O
MOS, local, inhalatory (devtox)	9.4E+09	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (devtox)	9.4E+09	[-]	O
MOS, local, total exposure (devtox)	364	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (devtox)	364	[-]	O
HUMAN HEALTH - RISK CHARACTERIZATION			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL [2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
MOS, local, inhalatory (repdose)	3.15E+06	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (repdose)	3.15E+06	[-]	O
MOS, local, total exposure (repdose)	2.8E+03	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (repdose)	2.8E+03	[-]	O
MOS, local, inhalatory (fert)	3.15E+06	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (fert)	3.15E+06	[-]	O
MOS, local, total exposure (fert)	2.8E+03	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (fert)	2.8E+03	[-]	O
MOS, local, inhalatory (mattox)	4.72E+05	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (mattox)	4.72E+05	[-]	O
MOS, local, total exposure (mattox)	420	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (mattox)	420	[-]	O
MOS, local, inhalatory (devtox)	4.72E+05	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (devtox)	4.72E+05	[-]	O
MOS, local, total exposure (devtox)	420	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (devtox)	420	[-]	O

Name	Value	Units	Status
HUMAN HEALTH - RISK CHARACTERIZATION			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL [3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
MOS, local, inhalatory (repdose)	3.06E+06	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (repdose)	3.06E+06	[-]	O
MOS, local, total exposure (repdose)	9.05E+03	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (repdose)	9.05E+03	[-]	O
MOS, local, inhalatory (fert)	3.06E+06	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (fert)	3.06E+06	[-]	O
MOS, local, total exposure (fert)	9.05E+03	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (fert)	9.05E+03	[-]	O
MOS, local, inhalatory (mattox)	4.6E+05	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (mattox)	4.6E+05	[-]	O
MOS, local, total exposure (mattox)	1.36E+03	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (mattox)	1.36E+03	[-]	O
MOS, local, inhalatory (devtox)	4.6E+05	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (devtox)	4.6E+05	[-]	O
MOS, local, total exposure (devtox)	1.36E+03	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (devtox)	1.36E+03	[-]	O
HUMAN HEALTH - RISK CHARACTERIZATION			
HUMANS EXPOSED VIA THE ENVIRONMENT			
REGIONAL			
MOS, regional, inhalatory (repdose)	4.27E+11	[-]	O
Ratio MOS/Ref-MOS, regional, inhalatory (repdose)	4.27E+11	[-]	O
MOS, regional, total exposure (repdose)	1.38E+08	[-]	O
Ratio MOS/Ref-MOS, regional, total exposure (repdose)	1.38E+08	[-]	O
MOS, regional, inhalatory (fert)	4.27E+11	[-]	O
Ratio MOS/Ref-MOS, regional, inhalatory (fert)	4.27E+11	[-]	O
MOS, regional, total exposure (fert)	1.38E+08	[-]	O
Ratio MOS/Ref-MOS, regional, total exposure (fert)	1.38E+08	[-]	O
MOS, regional, inhalatory (mattox)	6.4E+10	[-]	O
Ratio MOS/Ref-MOS, regional, inhalatory (mattox)	6.4E+10	[-]	O
MOS, regional, total exposure (mattox)	2.07E+07	[-]	O
Ratio MOS/Ref-MOS, regional, total exposure (mattox)	2.07E+07	[-]	O
MOS, regional, inhalatory (devtox)	6.4E+10	[-]	O
Ratio MOS/Ref-MOS, regional, inhalatory (devtox)	6.4E+10	[-]	O
MOS, regional, total exposure (devtox)	2.07E+07	[-]	O
Ratio MOS/Ref-MOS, regional, total exposure (devtox)	2.07E+07	[-]	O

EUSES 2 Summary report	Single substance
Printed on	15-12-2017 17:06:16
Study	TFA 2100 Plateau, mid EC50
Substance	Trifluoroacetic acid
Defaults	Standard Euses 2.1
Assessment types	1A, 1B, 2, 3A, 3B
Base set complete	No
Explanation status column	O = Output; D = Default; S = Set; I = Imported

Name	Value	Units	Status
IDENTIFICATION OF THE SUBSTANCE			
General name	Trifluoroacetic acid		S
CAS-No	76-05-1		S
EC-notification no.	200-929-3		S
EINECS no.	200-929-3		S
Molecular weight	114.02	[g.mol-1]	S

Printed on	15-12-2017 17:06:16
Study	Trifluoroacetic acid
Substance	TFA 2100 Plateau, mid EC50
Defaults	Standard Euses 2.1
Assessment types	1A, 1B, 2, 3A, 3B
Base set complete	No

Name	Value	Units	Status
PHYSICO-CHEMICAL PROPERTIES			
Melting point	-15.2	[oC]	S
Boiling point	71.78	[oC]	S
Vapour pressure at test temperature	1.58E+04	[Pa]	S
Vapour pressure at 25 [oC]	1.58E+04	[Pa]	O
Water solubility at test temperature	1E+05	[mg.l-1]	S
Water solubility at 25 [oC]	1E+05	[mg.l-1]	O
Octanol-water partition coefficient	-0.2	[log10]	S
Henry's law constant at 25 [oC]	7.13E-03	[Pa.m3.mol-1]	S

Name	Value	Units	Status
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
Tonnage of substance in Europe	1.2E+05	[tonnes.yr-1]	O
Regional production volume of substance	1E+05	[tonnes.yr-1]	O
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
[1 "CHEMICAL PRODUCTION", IC=3/UC=29]			
Industry category	3 Chemical industry: chemicals used in synthesis		S
Use category	29 Heat transferring agents		S
Fraction of tonnage for application	100	[%]	O
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
[PRODUCTION]			
Use specific emission scenario	No		D
Emission tables	A1.1 (general table), B1.6 (general table)		S
Emission scenario	no special scenario selected/available		S
Main category production	Ib Intermed. stored on-site/continuous prod.		S
Fraction of tonnage released to air	0.95	[-]	S
Fraction of tonnage released to wastewater	1.5E-03	[-]	S
Fraction of tonnage released to surface water	0.015	[-]	S
Fraction of tonnage released to industrial soil	0.015	[-]	S
Fraction of tonnage released to agricultural soil	0.015	[-]	S
Fraction of the main local source	0.1	[-]	S
Number of emission days per year	300	[-]	O
Local emission to air during episode	1.4815E+04	[kg.d-1]	S
Local emission to wastewater during episode	150	[kg.d-1]	S
Intermittent release	Yes		S
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
[2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29]			
Industry category	5 Personal / domestic use		S
Use category	29 Heat transferring agents		S
Fraction of tonnage for application	65	[%]	S
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
[PRIVATE USE]			
Use specific emission scenario	No		D
Emission tables	A4.1 (specific uses), B4.1 (general table)		S
Emission scenario	no special scenario selected/available		S
Fraction of tonnage released to air	0.95	[-]	S
Fraction of tonnage released to wastewater	5E-03	[-]	S
Fraction of tonnage released to surface water	0.015	[-]	S
Fraction of tonnage released to industrial soil	0.015	[-]	S
Fraction of tonnage released to agricultural soil	0.015	[-]	S
Fraction of the main local source	0.65	[-]	S
Number of emission days per year	365	[-]	O
Local emission to air during episode	2	[kg.d-1]	S
Local emission to wastewater during episode	226	[kg.d-1]	O
Intermittent release	No		D
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
[3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29]			
Industry category	6 Public domain		S
Use category	29 Heat transferring agents		S
Fraction of tonnage for application	0.35	[-]	S

Printed on	15-12-2017 17:06:16
Study	Trifluoroacetic acid
Substance	TFA 2100 Plateau, mid EC50
Defaults	Standard Euses 2.1
Assessment types	1A, 1B, 2, 3A, 3B
Base set complete	No

Name	Value	Units	Status
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
[INDUSTRIAL USE]			
Use specific emission scenario	No		D
Emission tables	A3.5 (specific uses), B3.3 (specific uses)		S
Emission scenario	no special scenario selected/available		S
Fraction of tonnage released to air	0.95	[-]	S
Fraction of tonnage released to wastewater	5E-03	[-]	S
Fraction of tonnage released to surface water	0.015	[-]	S
Fraction of tonnage released to industrial soil	0.015	[-]	S
Fraction of tonnage released to agricultural soil	0.015	[-]	S
Fraction of the main local source	0.35	[-]	S
Number of emission days per year	50	[-]	O
Local emission to air during episode	15	[kg.d-1]	S
Local emission to wastewater during episode	478	[kg.d-1]	O
Intermittent release	No		D
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
TOTAL REGIONAL EMISSIONS TO COMPARTMENTS			
Total regional emission to air	1.07116E+05	[kg.d-1]	S
Total regional emission to wastewater	1.0711E+04	[kg.d-1]	S
Total regional emission to surface water	5.3558E+04	[kg.d-1]	S
Total regional emission to industrial soil	2.1423E+04	[kg.d-1]	S
Total regional emission to agricultural soil	2.1423E+04	[kg.d-1]	S
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
TOTAL CONTINENTAL EMISSIONS TO COMPARTMENTS			
Total continental emission to air	3.21349E+05	[kg.d-1]	S
Total continental emission to wastewater	3.2134E+04	[kg.d-1]	S
Total continental emission to surface water	1.60674E+05	[kg.d-1]	S
Total continental emission to industrial soil	6.4269E+04	[kg.d-1]	S
Total continental emission to agricultural soil	6.4269E+04	[kg.d-1]	S
ENVIRONMENT-EXPOSURE			
PARTITION COEFFICIENTS			
Organic carbon-water partition coefficient	1	[l.kg-1]	S
ENVIRONMENT-EXPOSURE			
DEGRADATION AND TRANSFORMATION			
Characterization of biodegradability	Not biodegradable		S
Degradation calculation method in STP	First order, standard OECD/EU tests		D
Rate constant for biodegradation in STP	0	[d-1]	O
Rate constant for biodegradation in surface water	0	[d-1] (12[oC])	O
Rate constant for biodegradation in bulk soil	6.93E-07	[d-1] (12[oC])	O
Rate constant for biodegradation in aerated sediment	6.93E-07	[d-1] (12[oC])	O
Rate constant for hydrolysis in surface water	6.93E-07	[d-1] (12[oC])	O
Rate constant for photolysis in surface water	6.93E-07	[d-1]	O
ENVIRONMENT-EXPOSURE			
SEWAGE TREATMENT			
LOCAL STP [1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
OUTPUT			
Fraction of emission directed to air by STP	6.83E-03	[%]	O
Fraction of emission directed to water by STP	100	[%]	O
Fraction of emission directed to sludge by STP	0.0125	[%]	O
Fraction of the emission degraded in STP	0	[%]	O
Concentration in untreated wastewater	7.5E+04	[ug.l-1]	O
Concentration of chemical (total) in the STP-effluent	75	[mg.l-1]	O
Concentration in effluent exceeds solubility	No		O
Concentration in dry sewage sludge	23.8	[mg.kg-1]	O
PEC for micro-organisms in the STP	75	[mg.l-1]	O

Name	Value	Units	Status
ENVIRONMENT-EXPOSURE			
SEWAGE TREATMENT			
LOCAL STP [2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
OUTPUT			
Fraction of emission directed to air by STP	6.83E-03	[%]	O
Fraction of emission directed to water by STP	100	[%]	O
Fraction of emission directed to sludge by STP	0.0125	[%]	O
Fraction of the emission degraded in STP	0	[%]	O
Concentration in untreated wastewater	113	[mg.l-1]	O
Concentration of chemical (total) in the STP-effluent	113	[mg.l-1]	O
Concentration in effluent exceeds solubility	No		O
Concentration in dry sewage sludge	35.8	[mg.kg-1]	O
PEC for micro-organisms in the STP	113	[mg.l-1]	O
ENVIRONMENT-EXPOSURE			
SEWAGE TREATMENT			
LOCAL STP [3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
OUTPUT			
Fraction of emission directed to air by STP	6.83E-03	[%]	O
Fraction of emission directed to water by STP	100	[%]	O
Fraction of emission directed to sludge by STP	0.0125	[%]	O
Fraction of the emission degraded in STP	0	[%]	O
Concentration in untreated wastewater	239	[mg.l-1]	O
Concentration of chemical (total) in the STP-effluent	239	[mg.l-1]	O
Concentration in effluent exceeds solubility	No		O
Concentration in dry sewage sludge	75.7	[mg.kg-1]	O
PEC for micro-organisms in the STP	239	[mg.l-1]	O
ENVIRONMENT-EXPOSURE			
SEWAGE TREATMENT			
REGIONAL STP			
Fraction of emission directed to air	10	[%]	S
Fraction of emission directed to water	90	[%]	S
ENVIRONMENT-EXPOSURE			
SEWAGE TREATMENT			
CONTINENTAL STP			
Fraction of emission directed to air	10	[%]	S
Fraction of emission directed to water	90	[%]	S
Fraction of the emission degraded	0	[%]	S
ENVIRONMENT-EXPOSURE			
DISTRIBUTION			
LOCAL SCALE			
DEFAULT VALUES FOR LOCAL SCALE			
Calculate dilution from river flow rate	No		S
ENVIRONMENT-EXPOSURE			
DISTRIBUTION			
LOCAL SCALE			
[1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
Concentration in air during emission episode	2.9E-08	[mg.m-3]	S
Annual average concentration in air, 100 m from point source	2.38E-08	[mg.m-3]	O
Concentration in surface water during emission episode (dissolved)	7.5	[mg.l-1]	O
Annual average concentration in surface water (dissolved)	6.16	[mg.l-1]	O
Local PEC in surface water during emission episode (dissolved)	7.5	[mg.l-1]	O
Annual average local PEC in surface water (dissolved)	6.16	[mg.l-1]	O
Local PEC in fresh-water sediment during emission episode	6.03	[mg.kgwwt-1]	O
Concentration in seawater during emission episode (dissolved)	0.75	[mg.l-1]	O
Annual average concentration in seawater (dissolved)	0.616	[mg.l-1]	O
Local PEC in seawater during emission episode (dissolved)	0.75	[mg.l-1]	O
Annual average local PEC in seawater (dissolved)	0.617	[mg.l-1]	O
Local PEC in marine sediment during emission episode	0.603	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 30 days	1.45	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 180 days	1.43	[mg.kgwwt-1]	O
Local PEC in grassland (total) averaged over 180 days	1.42	[mg.kgwwt-1]	O
Local PEC in groundwater under agricultural soil	10.6	[mg.l-1]	O

Name	Value	Units	Status
ENVIRONMENT-EXPOSURE			
DISTRIBUTION			
LOCAL SCALE			
[2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
Concentration in air during emission episode	5.56E-04	[mg.m-3]	O
Annual average concentration in air, 100 m from point source	5.56E-04	[mg.m-3]	O
Concentration in surface water during emission episode (dissolved)	11.3	[mg.l-1]	O
Annual average concentration in surface water (dissolved)	11.3	[mg.l-1]	O
Local PEC in surface water during emission episode (dissolved)	11.3	[mg.l-1]	O
Annual average local PEC in surface water (dissolved)	11.3	[mg.l-1]	O
Local PEC in fresh-water sediment during emission episode	9.1	[mg.kgwwt-1]	O
Concentration in seawater during emission episode (dissolved)	1.13	[mg.l-1]	O
Annual average concentration in seawater (dissolved)	1.13	[mg.l-1]	O
Local PEC in seawater during emission episode (dissolved)	1.13	[mg.l-1]	O
Annual average local PEC in seawater (dissolved)	1.13	[mg.l-1]	O
Local PEC in marine sediment during emission episode	0.91	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 30 days	0.0495	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 180 days	0.0262	[mg.kgwwt-1]	O
Local PEC in grassland (total) averaged over 180 days	9.81E-03	[mg.kgwwt-1]	O
Local PEC in groundwater under agricultural soil	0.194	[mg.l-1]	O
ENVIRONMENT-EXPOSURE			
DISTRIBUTION			
LOCAL SCALE			
[3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
Concentration in air during emission episode	4.17E-03	[mg.m-3]	O
Annual average concentration in air, 100 m from point source	5.71E-04	[mg.m-3]	O
Concentration in surface water during emission episode (dissolved)	23.9	[mg.l-1]	O
Annual average concentration in surface water (dissolved)	3.27	[mg.l-1]	O
Local PEC in surface water during emission episode (dissolved)	23.9	[mg.l-1]	O
Annual average local PEC in surface water (dissolved)	3.27	[mg.l-1]	O
Local PEC in fresh-water sediment during emission episode	19.2	[mg.kgwwt-1]	O
Concentration in seawater during emission episode (dissolved)	2.39	[mg.l-1]	O
Annual average concentration in seawater (dissolved)	0.327	[mg.l-1]	O
Local PEC in seawater during emission episode (dissolved)	2.39	[mg.l-1]	O
Annual average local PEC in seawater (dissolved)	0.327	[mg.l-1]	O
Local PEC in marine sediment during emission episode	1.92	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 30 days	0.0988	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 180 days	0.0495	[mg.kgwwt-1]	O
Local PEC in grassland (total) averaged over 180 days	0.0149	[mg.kgwwt-1]	O
Local PEC in groundwater under agricultural soil	0.366	[mg.l-1]	O
ENVIRONMENT-EXPOSURE			
DISTRIBUTION			
REGIONAL AND CONTINENTAL SCALE			
CONTINENTAL			
Continental PEC in surface water (dissolved)	8.17E-03	[mg.l-1]	O
Continental PEC in seawater (dissolved)	2.2E-03	[mg.l-1]	O
Continental PEC in air (total)	8.38E-03	[mg.m-3]	O
Continental PEC in agricultural soil (total)	3.41E-03	[mg.kgwwt-1]	O
Continental PEC in pore water of agricultural soils	0.0251	[mg.l-1]	O
Continental PEC in natural soil (total)	5.21E-04	[mg.kgwwt-1]	O
Continental PEC in industrial soil (total)	0.0179	[mg.kgwwt-1]	O
Continental PEC in sediment (total)	5.72E-03	[mg.kgwwt-1]	O
Continental PEC in seawater sediment (total)	1.56E-03	[mg.kgwwt-1]	O

Printed on	15-12-2017 17:06:16
Study	Trifluoroacetic acid
Substance	TFA 2100 Plateau, mid EC50
Defaults	Standard Euses 2.1
Assessment types	1A, 1B, 2, 3A, 3B
Base set complete	No

Name	Value	Units	Status
ENVIRONMENT-EXPOSURE			
DISTRIBUTION			
REGIONAL AND CONTINENTAL SCALE			
REGIONAL			
Regional PEC in surface water (dissolved)	3.28E-04	[mg.l-1]	S
Regional PEC in seawater (dissolved)	2E-04	[mg.l-1]	S
Regional PEC in air (total)	4.1E-09	[mg.m-3]	S
Regional PEC in agricultural soil (total)	5E-03	[mg.kgwwt-1]	S
Regional PEC in pore water of agricultural soils	3.28E-04	[mg.l-1]	S
Regional PEC in natural soil (total)	5E-03	[mg.kgwwt-1]	S
Regional PEC in industrial soil (total)	5E-03	[mg.kgwwt-1]	S
Regional PEC in sediment (total)	5E-03	[mg.kgwwt-1]	S
Regional PEC in seawater sediment (total)	5E-03	[mg.kgwwt-1]	S
ENVIRONMENT-EXPOSURE			
BIOCONCENTRATION			
Bioconcentration factor for earthworms	0.848	[l.kgwwt-1]	O
Bioconcentration factor for fish	1.41	[l.kgwwt-1]	O
ENVIRONMENT-EXPOSURE			
SECONDARY POISONING [1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
Concentration in fish for secondary poisoning (freshwater)	4.35	[mg.kgwwt-1]	O
Concentration in fish for secondary poisoning (marine)	0.436	[mg.kgwwt-1]	O
Concentration in fish-eating marine top-predators	0.0873	[mg.kgwwt-1]	O
Concentration in earthworms from agricultural soil	4.11	[mg.kg-1]	O
ENVIRONMENT-EXPOSURE			
SECONDARY POISONING [2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
Concentration in fish for secondary poisoning (freshwater)	7.99	[mg.kgwwt-1]	O
Concentration in fish for secondary poisoning (marine)	0.799	[mg.kgwwt-1]	O
Concentration in fish-eating marine top-predators	0.16	[mg.kgwwt-1]	O
Concentration in earthworms from agricultural soil	0.0754	[mg.kg-1]	O
ENVIRONMENT-EXPOSURE			
SECONDARY POISONING [3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
Concentration in fish for secondary poisoning (freshwater)	2.31	[mg.kgwwt-1]	O
Concentration in fish for secondary poisoning (marine)	0.231	[mg.kgwwt-1]	O
Concentration in fish-eating marine top-predators	0.0465	[mg.kgwwt-1]	O
Concentration in earthworms from agricultural soil	0.142	[mg.kg-1]	O

Name	Value	Units	Status
ENVIRONMENT - EFFECTS			
MICRO-ORGANISMS			
Test system	Respiration inhibition, EU Annex V C.11, OECD 209	D	
EC50 for micro-organisms in a STP	832	[mg.l-1]	S
EC10 for micro-organisms in a STP	832	[mg.l-1]	S
NOEC for micro-organisms in a STP	832	[mg.l-1]	S
PNEC for micro-organisms in a STP	8.32	[mg.l-1]	O
Assessment factor applied in extrapolation to PNEC micro	10	[-]	S
ENVIRONMENT - EFFECTS			
FRESH_WATER ORGANISMS			
LC50 for fish	1.2E+03	[mg.l-1]	S
L(E)C50 for Daphnia	1.2E+03	[mg.l-1]	S
EC50 for algae	99	[mg.l-1]	S
LC50 for additional taxonomic group	??	[mg.l-1]	D
NOEC for fish	??	[mg.l-1]	D
NOEC for Daphnia	??	[mg.l-1]	D
NOEC for algae	??	[mg.l-1]	D
NOEC for additional taxonomic group	??	[mg.l-1]	D
PNEC for aquatic organisms	0.099	[mg.l-1]	O
PNEC for aquatic organisms, intermittent releases	0.99	[mg.l-1]	O
ENVIRONMENT - EFFECTS			
MARINE ORGANISMS			
LC50 for fish (marine)	??	[mg.l-1]	D
L(E)C50 for crustaceans (marine)	??	[mg.l-1]	D
EC50 for algae (marine)	103	[mg.l-1]	S
LC50 for additional taxonomic group (marine)	??	[mg.l-1]	D
NOEC for fish (marine)	??	[mg.l-1]	D
NOEC for crustaceans (marine)	??	[mg.l-1]	D
NOEC for algae (marine)	??	[mg.l-1]	D
NOEC for additional taxonomic group (marine)	??	[mg.l-1]	D
PNEC for marine organisms	9.9E-03	[mg.l-1]	O
ENVIRONMENT - EFFECTS			
FRESH-WATER SEDIMENT ORGANISMS			
LC50 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
PNEC for fresh-water sediment, normalised to 5% o.c. (regional)	0.0796	[mg.kgwwt-1]	O
ENVIRONMENT - EFFECTS			
MARINE SEDIMENT ORGANISMS			
LC50 for marine sediment organism	??	[mg.kgwwt-1]	D
EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D
PNEC for marine sediment, normalised to 5% o.c. (regional)	7.96E-03	[mg.kgwwt-1]	O

Name	Value	Units	Status
ENVIRONMENT - EFFECTS			
TERRESTRIAL ORGANISMS			
LC50 for plants	250	[mg.kgdwt-1]	S
LC50 for earthworms	??	[mg.kgwwt-1]	D
EC50 for microorganisms	??	[mg.kgwwt-1]	D
LC50 for other terrestrial species	??	[mg.kgwwt-1]	D
NOEC for plants	??	[mg.kgwwt-1]	D
NOEC for earthworms	??	[mg.kgwwt-1]	D
NOEC for microorganisms	??	[mg.kgwwt-1]	D
NOEC for additional taxonomic group	??	[mg.kgwwt-1]	D
NOEC for additional taxonomic group	??	[mg.kgwwt-1]	D
PNEC for terrestrial organisms	0.0134	[mg.kgwwt-1]	O
Equilibrium partitioning used for PNEC in soil?	Yes		O
ENVIRONMENT - EFFECTS			
BIRDS AND MAMMALS			
Oral NOAEL (repdose)	1E+03	[mg.kg-1.d-1]	S
NOEC via food (repdose)	1E+04	[mg.kg-1]	O
Inhalatory NOAEL (repdose)	1.75E+03	[mg.m-3]	O
Dermal NOAEL (repdose)	1E+03	[mg.kg-1.d-1]	O
Oral NOAEL (fert)	1E+03	[mg.kg-1.d-1]	S
NOEC via food (fert)	1E+04	[mg.kg-1]	O
Inhalatory NOAEL (fert)	1.75E+03	[mg.m-3]	O
Dermal NOAEL (fert)	1E+03	[mg.kg-1.d-1]	O
Oral NOAEL (mattox)	150	[mg.kg-1.d-1]	S
NOEC via food (mattox)	1.5E+03	[mg.kg-1]	O
Inhalatory NOAEL (mattox)	262	[mg.m-3]	O
Dermal NOAEL (mattox)	150	[mg.kg-1.d-1]	O
Oral NOAEL (devtox)	150	[mg.kg-1.d-1]	S
NOEC via food (devtox)	1.5E+03	[mg.kg-1]	O
Inhalatory NOAEL (devtox)	262	[mg.m-3]	O
Dermal NOAEL (devtox)	150	[mg.kg-1.d-1]	O
Duration of (sub-)chronic oral test	28 days		D
NOEC via food for secondary poisoning	1E+04	[mg.kg-1]	O
PNEC for secondary poisoning of birds and mammals	33.3	[mg.kg-1]	O

Name	Value	Units	Status
ENVIRONMENT - RISK CHARACTERIZATION			
LOCAL [1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
RCR for the local fresh-water compartment	7.57	[-]	O
RCR for the local fresh-water compartment, statistical method	??	[-]	O
RCR for the local marine compartment	75.8	[-]	O
RCR for the local marine compartment, statistical method	??	[-]	O
RCR for the local fresh-water sediment compartment	75.7	[-]	O
RCR for the local marine sediment compartment	75.8	[-]	O
RCR for the local soil compartment	108	[-]	O
RCR for the local soil compartment, statistical method	??	[-]	O
RCR for the sewage treatment plant	9.01	[-]	O
RCR for fish-eating birds and mammals (fresh-water)	0.131	[-]	O
RCR for fish-eating birds and mammals (marine)	0.0131	[-]	O
RCR for top predators (marine)	2.62E-03	[-]	O
RCR for worm-eating birds and mammals	0.123	[-]	O
ENVIRONMENT - RISK CHARACTERIZATION			
LOCAL [2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
RCR for the local fresh-water compartment	114	[-]	O
RCR for the local fresh-water compartment, statistical method	??	[-]	O
RCR for the local marine compartment	114	[-]	O
RCR for the local marine compartment, statistical method	??	[-]	O
RCR for the local fresh-water sediment compartment	114	[-]	O
RCR for the local marine sediment compartment	114	[-]	O
RCR for the local soil compartment	3.7	[-]	O
RCR for the local soil compartment, statistical method	??	[-]	O
RCR for the sewage treatment plant	13.6	[-]	O
RCR for fish-eating birds and mammals (fresh-water)	0.24	[-]	O
RCR for fish-eating birds and mammals (marine)	0.024	[-]	O
RCR for top predators (marine)	4.8E-03	[-]	O
RCR for worm-eating birds and mammals	2.26E-03	[-]	O
ENVIRONMENT - RISK CHARACTERIZATION			
LOCAL [3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
RCR for the local fresh-water compartment	241	[-]	O
RCR for the local fresh-water compartment, statistical method	??	[-]	O
RCR for the local marine compartment	241	[-]	O
RCR for the local marine compartment, statistical method	??	[-]	O
RCR for the local fresh-water sediment compartment	241	[-]	O
RCR for the local marine sediment compartment	241	[-]	O
RCR for the local soil compartment	7.37	[-]	O
RCR for the local soil compartment, statistical method	??	[-]	O
RCR for the sewage treatment plant	28.7	[-]	O
RCR for fish-eating birds and mammals (fresh-water)	0.0693	[-]	O
RCR for fish-eating birds and mammals (marine)	6.94E-03	[-]	O
RCR for top predators (marine)	1.4E-03	[-]	O
RCR for worm-eating birds and mammals	4.27E-03	[-]	O
ENVIRONMENT - RISK CHARACTERIZATION			
REGIONAL			
RCR for the regional fresh-water compartment	3.31E-03	[-]	O
RCR for the regional fresh-water compartment, statistical method	??	[-]	O
RCR for the regional marine compartment	0.0202	[-]	O
RCR for the regional marine compartment, statistical method	??	[-]	O
RCR for the regional fresh-water sediment compartment	0.0628	[-]	O
RCR for the regional marine sediment compartment	0.628	[-]	O
RCR for the regional soil compartment	0.373	[-]	O
RCR for the regional soil compartment, statistical method	??	[-]	O

Name	Value	Units	Status
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
Purification factor for surface water	1	[-]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
CONCENTRATIONS IN INTAKE MEDIA [1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
Local concentration in wet fish	8.71	[mg.kg-1]	O
Local concentration in root tissue of plant	9.94	[mg.kg-1]	O
Local concentration in leaves of plant	2.34	[mg.kg-1]	O
Local concentration in grass (wet weight)	2.32	[mg.kg-1]	O
Local concentration in drinking water	10.6	[mg.l-1]	O
Local concentration in meat (wet weight)	5.88E-04	[mg.kg-1]	O
Local concentration in milk (wet weight)	5.88E-03	[mg.kg-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
DOSES IN INTAKE MEDIA [1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
Daily dose through intake of drinking water	0.303	[mg.kg-1.d-1]	O
Daily dose through intake of fish	0.0143	[mg.kg-1.d-1]	O
Daily dose through intake of leaf crops	0.0401	[mg.kg-1.d-1]	O
Daily dose through intake of root crops	0.0545	[mg.kg-1.d-1]	O
Daily dose through intake of meat	2.53E-06	[mg.kg-1.d-1]	O
Daily dose through intake of milk	4.72E-05	[mg.kg-1.d-1]	O
Daily dose through intake of air	7.98E-09	[mg.kg-1.d-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
FRACTIONS OF TOTAL DOSE [1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
Fraction of total dose through intake of drinking water	0.735	[-]	O
Fraction of total dose through intake of fish	0.0347	[-]	O
Fraction of total dose through intake of leaf crops	0.0973	[-]	O
Fraction of total dose through intake of root crops	0.132	[-]	O
Fraction of total dose through intake of meat	6.14E-06	[-]	O
Fraction of total dose through intake of milk	1.14E-04	[-]	O
Fraction of total dose through intake of air	1.94E-08	[-]	O
Local total daily intake for humans	0.412	[mg.kg-1.d-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
CONCENTRATIONS IN INTAKE MEDIA [2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
Local concentration in wet fish	16	[mg.kg-1]	O
Local concentration in root tissue of plant	0.182	[mg.kg-1]	O
Local concentration in leaves of plant	0.38	[mg.kg-1]	O
Local concentration in grass (wet weight)	0.353	[mg.kg-1]	O
Local concentration in drinking water	11.3	[mg.l-1]	O
Local concentration in meat (wet weight)	5.13E-04	[mg.kg-1]	O
Local concentration in milk (wet weight)	5.13E-03	[mg.kg-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
DOSES IN INTAKE MEDIA [2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
Daily dose through intake of drinking water	0.323	[mg.kg-1.d-1]	O
Daily dose through intake of fish	0.0262	[mg.kg-1.d-1]	O
Daily dose through intake of leaf crops	6.51E-03	[mg.kg-1.d-1]	O
Daily dose through intake of root crops	9.96E-04	[mg.kg-1.d-1]	O
Daily dose through intake of meat	2.21E-06	[mg.kg-1.d-1]	O
Daily dose through intake of milk	4.11E-05	[mg.kg-1.d-1]	O
Daily dose through intake of air	1.59E-04	[mg.kg-1.d-1]	O

Name	Value	Units	Status
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
FRACTIONS OF TOTAL DOSE [2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
Fraction of total dose through intake of drinking water	0.905	[-]	O
Fraction of total dose through intake of fish	0.0735	[-]	O
Fraction of total dose through intake of leaf crops	0.0182	[-]	O
Fraction of total dose through intake of root crops	2.79E-03	[-]	O
Fraction of total dose through intake of meat	6.18E-06	[-]	O
Fraction of total dose through intake of milk	1.15E-04	[-]	O
Fraction of total dose through intake of air	4.45E-04	[-]	O
Local total daily intake for humans	0.357	[mg.kg-1.d-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
CONCENTRATIONS IN INTAKE MEDIA [3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
Local concentration in wet fish	4.62	[mg.kg-1]	O
Local concentration in root tissue of plant	0.343	[mg.kg-1]	O
Local concentration in leaves of plant	0.427	[mg.kg-1]	O
Local concentration in grass (wet weight)	0.371	[mg.kg-1]	O
Local concentration in drinking water	3.27	[mg.l-1]	O
Local concentration in meat (wet weight)	1.63E-04	[mg.kg-1]	O
Local concentration in milk (wet weight)	1.63E-03	[mg.kg-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
DOSES IN INTAKE MEDIA [3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
Daily dose through intake of drinking water	0.0935	[mg.kg-1.d-1]	O
Daily dose through intake of fish	7.59E-03	[mg.kg-1.d-1]	O
Daily dose through intake of leaf crops	7.32E-03	[mg.kg-1.d-1]	O
Daily dose through intake of root crops	1.88E-03	[mg.kg-1.d-1]	O
Daily dose through intake of meat	7.01E-07	[mg.kg-1.d-1]	O
Daily dose through intake of milk	1.31E-05	[mg.kg-1.d-1]	O
Daily dose through intake of air	1.63E-04	[mg.kg-1.d-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
FRACTIONS OF TOTAL DOSE [3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
Fraction of total dose through intake of drinking water	0.846	[-]	O
Fraction of total dose through intake of fish	0.0687	[-]	O
Fraction of total dose through intake of leaf crops	0.0663	[-]	O
Fraction of total dose through intake of root crops	0.0171	[-]	O
Fraction of total dose through intake of meat	6.34E-06	[-]	O
Fraction of total dose through intake of milk	1.18E-04	[-]	O
Fraction of total dose through intake of air	1.48E-03	[-]	O
Local total daily intake for humans	0.11	[mg.kg-1.d-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
REGIONAL SCALE			
CONCENTRATIONS IN INTAKE MEDIA			
Regional concentration in wet fish	4.63E-04	[mg.kg-1]	O
Regional concentration in root tissue of plant	3.08E-04	[mg.kg-1]	O
Regional concentration in leaves of plant	7.48E-05	[mg.kg-1]	O
Regional concentration in grass (wet weight)	7.48E-05	[mg.kg-1]	O
Regional concentration in drinking water	1.23E-04	[mg.l-1]	S
Regional concentration in meat (wet weight)	1.12E-08	[mg.kg-1]	O
Regional concentration in milk (wet weight)	1.12E-07	[mg.kg-1]	O

Name	Value	Units	Status
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
REGIONAL SCALE			
DOSES IN INTAKE MEDIA			
Daily dose through intake of drinking water	3.51E-06	[mg.kg-1.d-1]	O
Daily dose through intake of fish	7.61E-07	[mg.kg-1.d-1]	O
Daily dose through intake of leaf crops	1.28E-06	[mg.kg-1.d-1]	O
Daily dose through intake of root crops	1.69E-06	[mg.kg-1.d-1]	O
Daily dose through intake of meat	4.83E-11	[mg.kg-1.d-1]	O
Daily dose through intake of milk	9.01E-10	[mg.kg-1.d-1]	O
Daily dose through intake of air	1.17E-09	[mg.kg-1.d-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
REGIONAL SCALE			
FRACTIONS OF TOTAL DOSE			
Fraction of total dose through intake of drinking water	0.485	[-]	O
Fraction of total dose through intake of fish	0.105	[-]	O
Fraction of total dose through intake of leaf crops	0.177	[-]	O
Fraction of total dose through intake of root crops	0.233	[-]	O
Fraction of total dose through intake of meat	6.67E-06	[-]	O
Fraction of total dose through intake of milk	1.24E-04	[-]	O
Fraction of total dose through intake of air	1.62E-04	[-]	O
Regional total daily intake for humans	7.25E-06	[mg.kg-1.d-1]	O

Name	Value	Units	Status
HUMAN HEALTH - RISK CHARACTERIZATION			
CURRENT CLASSIFICATION			
Corrosive (C, R34 or R35)	Yes		S
Irritating to skin (Xi, R38)	No		D
Irritating to eyes (Xi, R36)	No		D
Risk of serious damage to eyes (Xi, R41)	No		D
Irritating to respiratory system (Xi, R37)	No		D
May cause sensitisation by inhalation (Xn, R42)	No		D
May cause sensitisation by skin contact (Xi, R43)	No		D
May cause cancer (T, R45)	No		D
May cause cancer by inhalation (T, R49)	No		D
Possible risk of irreversible effects (Xn, R40)	No		D
HUMAN HEALTH - RISK CHARACTERIZATION			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL [1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
MOS, local, inhalatory (repdose)	6.26E+10	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (repdose)	6.26E+10	[-]	O
MOS, local, total exposure (repdose)	2.43E+03	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (repdose)	2.43E+03	[-]	O
MOS, local, inhalatory (fert)	6.26E+10	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (fert)	6.26E+10	[-]	O
MOS, local, total exposure (fert)	2.43E+03	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (fert)	2.43E+03	[-]	O
MOS, local, inhalatory (mattox)	9.4E+09	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (mattox)	9.4E+09	[-]	O
MOS, local, total exposure (mattox)	364	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (mattox)	364	[-]	O
MOS, local, inhalatory (devtox)	9.4E+09	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (devtox)	9.4E+09	[-]	O
MOS, local, total exposure (devtox)	364	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (devtox)	364	[-]	O
HUMAN HEALTH - RISK CHARACTERIZATION			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL [2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
MOS, local, inhalatory (repdose)	3.15E+06	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (repdose)	3.15E+06	[-]	O
MOS, local, total exposure (repdose)	2.8E+03	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (repdose)	2.8E+03	[-]	O
MOS, local, inhalatory (fert)	3.15E+06	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (fert)	3.15E+06	[-]	O
MOS, local, total exposure (fert)	2.8E+03	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (fert)	2.8E+03	[-]	O
MOS, local, inhalatory (mattox)	4.72E+05	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (mattox)	4.72E+05	[-]	O
MOS, local, total exposure (mattox)	420	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (mattox)	420	[-]	O
MOS, local, inhalatory (devtox)	4.72E+05	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (devtox)	4.72E+05	[-]	O
MOS, local, total exposure (devtox)	420	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (devtox)	420	[-]	O

Name	Value	Units	Status
HUMAN HEALTH - RISK CHARACTERIZATION			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL [3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
MOS, local, inhalatory (repdose)	3.06E+06	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (repdose)	3.06E+06	[-]	O
MOS, local, total exposure (repdose)	9.05E+03	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (repdose)	9.05E+03	[-]	O
MOS, local, inhalatory (fert)	3.06E+06	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (fert)	3.06E+06	[-]	O
MOS, local, total exposure (fert)	9.05E+03	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (fert)	9.05E+03	[-]	O
MOS, local, inhalatory (mattox)	4.6E+05	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (mattox)	4.6E+05	[-]	O
MOS, local, total exposure (mattox)	1.36E+03	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (mattox)	1.36E+03	[-]	O
MOS, local, inhalatory (devtox)	4.6E+05	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (devtox)	4.6E+05	[-]	O
MOS, local, total exposure (devtox)	1.36E+03	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (devtox)	1.36E+03	[-]	O
HUMAN HEALTH - RISK CHARACTERIZATION			
HUMANS EXPOSED VIA THE ENVIRONMENT			
REGIONAL			
MOS, regional, inhalatory (repdose)	4.27E+11	[-]	O
Ratio MOS/Ref-MOS, regional, inhalatory (repdose)	4.27E+11	[-]	O
MOS, regional, total exposure (repdose)	1.38E+08	[-]	O
Ratio MOS/Ref-MOS, regional, total exposure (repdose)	1.38E+08	[-]	O
MOS, regional, inhalatory (fert)	4.27E+11	[-]	O
Ratio MOS/Ref-MOS, regional, inhalatory (fert)	4.27E+11	[-]	O
MOS, regional, total exposure (fert)	1.38E+08	[-]	O
Ratio MOS/Ref-MOS, regional, total exposure (fert)	1.38E+08	[-]	O
MOS, regional, inhalatory (mattox)	6.4E+10	[-]	O
Ratio MOS/Ref-MOS, regional, inhalatory (mattox)	6.4E+10	[-]	O
MOS, regional, total exposure (mattox)	2.07E+07	[-]	O
Ratio MOS/Ref-MOS, regional, total exposure (mattox)	2.07E+07	[-]	O
MOS, regional, inhalatory (devtox)	6.4E+10	[-]	O
Ratio MOS/Ref-MOS, regional, inhalatory (devtox)	6.4E+10	[-]	O
MOS, regional, total exposure (devtox)	2.07E+07	[-]	O
Ratio MOS/Ref-MOS, regional, total exposure (devtox)	2.07E+07	[-]	O

EUSES 2 Summary report	Single substance
Printed on	15-12-2017 17:11:07
Study	TFA 2100 Plateau, high EC50
Substance	Trifluoroacetic acid
Defaults	Standard Euses 2.1
Assessment types	1A, 1B, 2, 3A, 3B
Base set complete	No
Explanation status column	O = Output; D = Default; S = Set; I = Imported

Name	Value	Units	Status
IDENTIFICATION OF THE SUBSTANCE			
General name	Trifluoroacetic acid		S
CAS-No	76-05-1		S
EC-notification no.	200-929-3		S
EINECS no.	200-929-3		S
Molecular weight	114.02	[g.mol-1]	S

Printed on	15-12-2017 17:11:07
Study	Trifluoroacetic acid
Substance	TFA 2100 Plateau, high EC50
Defaults	Standard Euses 2.1
Assessment types	1A, 1B, 2, 3A, 3B
Base set complete	No

Name	Value	Units	Status
PHYSICO-CHEMICAL PROPERTIES			
Melting point	-15.2	[oC]	S
Boiling point	71.78	[oC]	S
Vapour pressure at test temperature	1.58E+04	[Pa]	S
Vapour pressure at 25 [oC]	1.58E+04	[Pa]	O
Water solubility at test temperature	1E+05	[mg.l-1]	S
Water solubility at 25 [oC]	1E+05	[mg.l-1]	O
Octanol-water partition coefficient	-0.2	[log10]	S
Henry's law constant at 25 [oC]	7.13E-03	[Pa.m3.mol-1]	S

Printed on	15-12-2017 17:11:07
Study	Trifluoroacetic acid
Substance	TFA 2100 Plateau, high EC50
Defaults	Standard Euses 2.1
Assessment types	1A, 1B, 2, 3A, 3B
Base set complete	No

Name	Value	Units	Status
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
Tonnage of substance in Europe	1.2E+05	[tonnes.yr-1]	O
Regional production volume of substance	1E+05	[tonnes.yr-1]	O
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
[1 "CHEMICAL PRODUCTION", IC=3/UC=29]			
Industry category	3 Chemical industry: chemicals used in synthesis		S
Use category	29 Heat transferring agents		S
Fraction of tonnage for application	100	[%]	O
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
[PRODUCTION]			
Use specific emission scenario	No		D
Emission tables	A1.1 (general table), B1.6 (general table)		S
Emission scenario	no special scenario selected/available		S
Main category production	Ib Intermed. stored on-site/continuous prod.		S
Fraction of tonnage released to air	0.95	[-]	S
Fraction of tonnage released to wastewater	1.5E-03	[-]	S
Fraction of tonnage released to surface water	0.015	[-]	S
Fraction of tonnage released to industrial soil	0.015	[-]	S
Fraction of tonnage released to agricultural soil	0.015	[-]	S
Fraction of the main local source	0.1	[-]	S
Number of emission days per year	300	[-]	O
Local emission to air during episode	1.4815E+04	[kg.d-1]	S
Local emission to wastewater during episode	150	[kg.d-1]	S
Intermittent release	Yes		S
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
[2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29]			
Industry category	5 Personal / domestic use		S
Use category	29 Heat transferring agents		S
Fraction of tonnage for application	65	[%]	S
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
[PRIVATE USE]			
Use specific emission scenario	No		D
Emission tables	A4.1 (specific uses), B4.1 (general table)		S
Emission scenario	no special scenario selected/available		S
Fraction of tonnage released to air	0.95	[-]	S
Fraction of tonnage released to wastewater	5E-03	[-]	S
Fraction of tonnage released to surface water	0.015	[-]	S
Fraction of tonnage released to industrial soil	0.015	[-]	S
Fraction of tonnage released to agricultural soil	0.015	[-]	S
Fraction of the main local source	0.65	[-]	S
Number of emission days per year	365	[-]	O
Local emission to air during episode	2	[kg.d-1]	S
Local emission to wastewater during episode	226	[kg.d-1]	O
Intermittent release	No		D
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
[3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29]			
Industry category	6 Public domain		S
Use category	29 Heat transferring agents		S
Fraction of tonnage for application	0.35	[-]	S

Name	Value	Units	Status
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
[INDUSTRIAL USE]			
Use specific emission scenario	No		D
Emission tables	A3.5 (specific uses), B3.3 (specific uses)		S
Emission scenario	no special scenario selected/available		S
Fraction of tonnage released to air	0.95	[-]	S
Fraction of tonnage released to wastewater	5E-03	[-]	S
Fraction of tonnage released to surface water	0.015	[-]	S
Fraction of tonnage released to industrial soil	0.015	[-]	S
Fraction of tonnage released to agricultural soil	0.015	[-]	S
Fraction of the main local source	0.35	[-]	S
Number of emission days per year	50	[-]	O
Local emission to air during episode	15	[kg.d-1]	S
Local emission to wastewater during episode	478	[kg.d-1]	O
Intermittent release	No		D
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
TOTAL REGIONAL EMISSIONS TO COMPARTMENTS			
Total regional emission to air	1.07116E+05	[kg.d-1]	S
Total regional emission to wastewater	1.0711E+04	[kg.d-1]	S
Total regional emission to surface water	5.3558E+04	[kg.d-1]	S
Total regional emission to industrial soil	2.1423E+04	[kg.d-1]	S
Total regional emission to agricultural soil	2.1423E+04	[kg.d-1]	S
ENVIRONMENT-EXPOSURE			
RELEASE ESTIMATION			
TOTAL CONTINENTAL EMISSIONS TO COMPARTMENTS			
Total continental emission to air	3.21349E+05	[kg.d-1]	S
Total continental emission to wastewater	3.2134E+04	[kg.d-1]	S
Total continental emission to surface water	1.60674E+05	[kg.d-1]	S
Total continental emission to industrial soil	6.4269E+04	[kg.d-1]	S
Total continental emission to agricultural soil	6.4269E+04	[kg.d-1]	S
ENVIRONMENT-EXPOSURE			
PARTITION COEFFICIENTS			
Organic carbon-water partition coefficient	1	[l.kg-1]	S
ENVIRONMENT-EXPOSURE			
DEGRADATION AND TRANSFORMATION			
Characterization of biodegradability	Not biodegradable		S
Degradation calculation method in STP	First order, standard OECD/EU tests		D
Rate constant for biodegradation in STP	0	[d-1]	O
Rate constant for biodegradation in surface water	0	[d-1] (12[oC])	O
Rate constant for biodegradation in bulk soil	6.93E-07	[d-1] (12[oC])	O
Rate constant for biodegradation in aerated sediment	6.93E-07	[d-1] (12[oC])	O
Rate constant for hydrolysis in surface water	6.93E-07	[d-1] (12[oC])	O
Rate constant for photolysis in surface water	6.93E-07	[d-1]	O
ENVIRONMENT-EXPOSURE			
SEWAGE TREATMENT			
LOCAL STP [1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
OUTPUT			
Fraction of emission directed to air by STP	6.83E-03	[%]	O
Fraction of emission directed to water by STP	100	[%]	O
Fraction of emission directed to sludge by STP	0.0125	[%]	O
Fraction of the emission degraded in STP	0	[%]	O
Concentration in untreated wastewater	7.5E+04	[ug.l-1]	O
Concentration of chemical (total) in the STP-effluent	75	[mg.l-1]	O
Concentration in effluent exceeds solubility	No		O
Concentration in dry sewage sludge	23.8	[mg.kg-1]	O
PEC for micro-organisms in the STP	75	[mg.l-1]	O

Name	Value	Units	Status
ENVIRONMENT-EXPOSURE			
SEWAGE TREATMENT			
LOCAL STP [2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
OUTPUT			
Fraction of emission directed to air by STP	6.83E-03	[%]	O
Fraction of emission directed to water by STP	100	[%]	O
Fraction of emission directed to sludge by STP	0.0125	[%]	O
Fraction of the emission degraded in STP	0	[%]	O
Concentration in untreated wastewater	113	[mg.l-1]	O
Concentration of chemical (total) in the STP-effluent	113	[mg.l-1]	O
Concentration in effluent exceeds solubility	No		O
Concentration in dry sewage sludge	35.8	[mg.kg-1]	O
PEC for micro-organisms in the STP	113	[mg.l-1]	O
ENVIRONMENT-EXPOSURE			
SEWAGE TREATMENT			
LOCAL STP [3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
OUTPUT			
Fraction of emission directed to air by STP	6.83E-03	[%]	O
Fraction of emission directed to water by STP	100	[%]	O
Fraction of emission directed to sludge by STP	0.0125	[%]	O
Fraction of the emission degraded in STP	0	[%]	O
Concentration in untreated wastewater	239	[mg.l-1]	O
Concentration of chemical (total) in the STP-effluent	239	[mg.l-1]	O
Concentration in effluent exceeds solubility	No		O
Concentration in dry sewage sludge	75.7	[mg.kg-1]	O
PEC for micro-organisms in the STP	239	[mg.l-1]	O
ENVIRONMENT-EXPOSURE			
SEWAGE TREATMENT			
REGIONAL STP			
Fraction of emission directed to air	10	[%]	S
Fraction of emission directed to water	90	[%]	S
ENVIRONMENT-EXPOSURE			
SEWAGE TREATMENT			
CONTINENTAL STP			
Fraction of emission directed to air	10	[%]	S
Fraction of emission directed to water	90	[%]	S
Fraction of the emission degraded	0	[%]	S
ENVIRONMENT-EXPOSURE			
DISTRIBUTION			
LOCAL SCALE			
DEFAULT VALUES FOR LOCAL SCALE			
Calculate dilution from river flow rate	No		S
ENVIRONMENT-EXPOSURE			
DISTRIBUTION			
LOCAL SCALE			
[1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
Concentration in air during emission episode	2.9E-08	[mg.m-3]	S
Annual average concentration in air, 100 m from point source	2.38E-08	[mg.m-3]	O
Concentration in surface water during emission episode (dissolved)	7.5	[mg.l-1]	O
Annual average concentration in surface water (dissolved)	6.16	[mg.l-1]	O
Local PEC in surface water during emission episode (dissolved)	7.5	[mg.l-1]	O
Annual average local PEC in surface water (dissolved)	6.16	[mg.l-1]	O
Local PEC in fresh-water sediment during emission episode	6.03	[mg.kgwwt-1]	O
Concentration in seawater during emission episode (dissolved)	0.75	[mg.l-1]	O
Annual average concentration in seawater (dissolved)	0.616	[mg.l-1]	O
Local PEC in seawater during emission episode (dissolved)	0.75	[mg.l-1]	O
Annual average local PEC in seawater (dissolved)	0.617	[mg.l-1]	O
Local PEC in marine sediment during emission episode	0.603	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 30 days	1.45	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 180 days	1.43	[mg.kgwwt-1]	O
Local PEC in grassland (total) averaged over 180 days	1.42	[mg.kgwwt-1]	O
Local PEC in groundwater under agricultural soil	10.6	[mg.l-1]	O

Name	Value	Units	Status
ENVIRONMENT-EXPOSURE			
DISTRIBUTION			
LOCAL SCALE			
[2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
Concentration in air during emission episode	5.56E-04	[mg.m-3]	O
Annual average concentration in air, 100 m from point source	5.56E-04	[mg.m-3]	O
Concentration in surface water during emission episode (dissolved)	11.3	[mg.l-1]	O
Annual average concentration in surface water (dissolved)	11.3	[mg.l-1]	O
Local PEC in surface water during emission episode (dissolved)	11.3	[mg.l-1]	O
Annual average local PEC in surface water (dissolved)	11.3	[mg.l-1]	O
Local PEC in fresh-water sediment during emission episode	9.1	[mg.kgwwt-1]	O
Concentration in seawater during emission episode (dissolved)	1.13	[mg.l-1]	O
Annual average concentration in seawater (dissolved)	1.13	[mg.l-1]	O
Local PEC in seawater during emission episode (dissolved)	1.13	[mg.l-1]	O
Annual average local PEC in seawater (dissolved)	1.13	[mg.l-1]	O
Local PEC in marine sediment during emission episode	0.91	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 30 days	0.0495	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 180 days	0.0262	[mg.kgwwt-1]	O
Local PEC in grassland (total) averaged over 180 days	9.81E-03	[mg.kgwwt-1]	O
Local PEC in groundwater under agricultural soil	0.194	[mg.l-1]	O
ENVIRONMENT-EXPOSURE			
DISTRIBUTION			
LOCAL SCALE			
[3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
Concentration in air during emission episode	4.17E-03	[mg.m-3]	O
Annual average concentration in air, 100 m from point source	5.71E-04	[mg.m-3]	O
Concentration in surface water during emission episode (dissolved)	23.9	[mg.l-1]	O
Annual average concentration in surface water (dissolved)	3.27	[mg.l-1]	O
Local PEC in surface water during emission episode (dissolved)	23.9	[mg.l-1]	O
Annual average local PEC in surface water (dissolved)	3.27	[mg.l-1]	O
Local PEC in fresh-water sediment during emission episode	19.2	[mg.kgwwt-1]	O
Concentration in seawater during emission episode (dissolved)	2.39	[mg.l-1]	O
Annual average concentration in seawater (dissolved)	0.327	[mg.l-1]	O
Local PEC in seawater during emission episode (dissolved)	2.39	[mg.l-1]	O
Annual average local PEC in seawater (dissolved)	0.327	[mg.l-1]	O
Local PEC in marine sediment during emission episode	1.92	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 30 days	0.0988	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 180 days	0.0495	[mg.kgwwt-1]	O
Local PEC in grassland (total) averaged over 180 days	0.0149	[mg.kgwwt-1]	O
Local PEC in groundwater under agricultural soil	0.366	[mg.l-1]	O
ENVIRONMENT-EXPOSURE			
DISTRIBUTION			
REGIONAL AND CONTINENTAL SCALE			
CONTINENTAL			
Continental PEC in surface water (dissolved)	8.17E-03	[mg.l-1]	O
Continental PEC in seawater (dissolved)	2.2E-03	[mg.l-1]	O
Continental PEC in air (total)	8.38E-03	[mg.m-3]	O
Continental PEC in agricultural soil (total)	3.41E-03	[mg.kgwwt-1]	O
Continental PEC in pore water of agricultural soils	0.0251	[mg.l-1]	O
Continental PEC in natural soil (total)	5.21E-04	[mg.kgwwt-1]	O
Continental PEC in industrial soil (total)	0.0179	[mg.kgwwt-1]	O
Continental PEC in sediment (total)	5.72E-03	[mg.kgwwt-1]	O
Continental PEC in seawater sediment (total)	1.56E-03	[mg.kgwwt-1]	O

Name	Value	Units	Status
ENVIRONMENT-EXPOSURE			
DISTRIBUTION			
REGIONAL AND CONTINENTAL SCALE			
REGIONAL			
Regional PEC in surface water (dissolved)	3.28E-04	[mg.l-1]	S
Regional PEC in seawater (dissolved)	2E-04	[mg.l-1]	S
Regional PEC in air (total)	4.1E-09	[mg.m-3]	S
Regional PEC in agricultural soil (total)	5E-03	[mg.kgwwt-1]	S
Regional PEC in pore water of agricultural soils	3.28E-04	[mg.l-1]	S
Regional PEC in natural soil (total)	5E-03	[mg.kgwwt-1]	S
Regional PEC in industrial soil (total)	5E-03	[mg.kgwwt-1]	S
Regional PEC in sediment (total)	5E-03	[mg.kgwwt-1]	S
Regional PEC in seawater sediment (total)	5E-03	[mg.kgwwt-1]	S
ENVIRONMENT-EXPOSURE			
BIOCONCENTRATION			
Bioconcentration factor for earthworms	0.848	[l.kgwwt-1]	O
Bioconcentration factor for fish	1.41	[l.kgwwt-1]	O
ENVIRONMENT-EXPOSURE			
SECONDARY POISONING [1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
Concentration in fish for secondary poisoning (freshwater)	4.35	[mg.kgwwt-1]	O
Concentration in fish for secondary poisoning (marine)	0.436	[mg.kgwwt-1]	O
Concentration in fish-eating marine top-predators	0.0873	[mg.kgwwt-1]	O
Concentration in earthworms from agricultural soil	4.11	[mg.kg-1]	O
ENVIRONMENT-EXPOSURE			
SECONDARY POISONING [2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
Concentration in fish for secondary poisoning (freshwater)	7.99	[mg.kgwwt-1]	O
Concentration in fish for secondary poisoning (marine)	0.799	[mg.kgwwt-1]	O
Concentration in fish-eating marine top-predators	0.16	[mg.kgwwt-1]	O
Concentration in earthworms from agricultural soil	0.0754	[mg.kg-1]	O
ENVIRONMENT-EXPOSURE			
SECONDARY POISONING [3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
Concentration in fish for secondary poisoning (freshwater)	2.31	[mg.kgwwt-1]	O
Concentration in fish for secondary poisoning (marine)	0.231	[mg.kgwwt-1]	O
Concentration in fish-eating marine top-predators	0.0465	[mg.kgwwt-1]	O
Concentration in earthworms from agricultural soil	0.142	[mg.kg-1]	O

Name	Value	Units	Status
ENVIRONMENT - EFFECTS			
MICRO-ORGANISMS			
Test system	Respiration inhibition, EU Annex V C.11, OECD 209		D
EC50 for micro-organisms in a STP	832	[mg.l-1]	S
EC10 for micro-organisms in a STP	832	[mg.l-1]	S
NOEC for micro-organisms in a STP	832	[mg.l-1]	S
PNEC for micro-organisms in a STP	8.32	[mg.l-1]	O
Assessment factor applied in extrapolation to PNEC micro	10	[-]	S
ENVIRONMENT - EFFECTS			
FRESH_WATER ORGANISMS			
LC50 for fish	1.2E+03	[mg.l-1]	S
L(E)C50 for Daphnia	1.2E+03	[mg.l-1]	S
EC50 for algae	441	[mg.l-1]	S
LC50 for additional taxonomic group	??	[mg.l-1]	D
NOEC for fish	??	[mg.l-1]	D
NOEC for Daphnia	??	[mg.l-1]	D
NOEC for algae	??	[mg.l-1]	D
NOEC for additional taxonomic group	??	[mg.l-1]	D
PNEC for aquatic organisms	0.441	[mg.l-1]	O
PNEC for aquatic organisms, intermittent releases	4.41	[mg.l-1]	O
ENVIRONMENT - EFFECTS			
MARINE ORGANISMS			
LC50 for fish (marine)	??	[mg.l-1]	D
L(E)C50 for crustaceans (marine)	??	[mg.l-1]	D
EC50 for algae (marine)	732	[mg.l-1]	S
LC50 for additional taxonomic group (marine)	??	[mg.l-1]	D
NOEC for fish (marine)	??	[mg.l-1]	D
NOEC for crustaceans (marine)	??	[mg.l-1]	D
NOEC for algae (marine)	??	[mg.l-1]	D
NOEC for additional taxonomic group (marine)	??	[mg.l-1]	D
PNEC for marine organisms	0.0441	[mg.l-1]	O
ENVIRONMENT - EFFECTS			
FRESH-WATER SEDIMENT ORGANISMS			
LC50 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
PNEC for fresh-water sediment, normalised to 5% o.c. (regional)	0.355	[mg.kgwwt-1]	O
ENVIRONMENT - EFFECTS			
MARINE SEDIMENT ORGANISMS			
LC50 for marine sediment organism	??	[mg.kgwwt-1]	D
EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D
PNEC for marine sediment, normalised to 5% o.c. (regional)	0.0355	[mg.kgwwt-1]	O

Name	Value	Units	Status
ENVIRONMENT - EFFECTS			
TERRESTRIAL ORGANISMS			
LC50 for plants	250	[mg.kgdwt-1]	S
LC50 for earthworms	??	[mg.kgwwt-1]	D
EC50 for microorganisms	??	[mg.kgwwt-1]	D
LC50 for other terrestrial species	??	[mg.kgwwt-1]	D
NOEC for plants	??	[mg.kgwwt-1]	D
NOEC for earthworms	??	[mg.kgwwt-1]	D
NOEC for microorganisms	??	[mg.kgwwt-1]	D
NOEC for additional taxonomic group	??	[mg.kgwwt-1]	D
NOEC for additional taxonomic group	??	[mg.kgwwt-1]	D
PNEC for terrestrial organisms	0.0597	[mg.kgwwt-1]	O
Equilibrium partitioning used for PNEC in soil?	Yes		O
ENVIRONMENT - EFFECTS			
BIRDS AND MAMMALS			
Oral NOAEL (repdose)	1E+03	[mg.kg-1.d-1]	S
NOEC via food (repdose)	1E+04	[mg.kg-1]	O
Inhalatory NOAEL (repdose)	1.75E+03	[mg.m-3]	O
Dermal NOAEL (repdose)	1E+03	[mg.kg-1.d-1]	O
Oral NOAEL (fert)	1E+03	[mg.kg-1.d-1]	S
NOEC via food (fert)	1E+04	[mg.kg-1]	O
Inhalatory NOAEL (fert)	1.75E+03	[mg.m-3]	O
Dermal NOAEL (fert)	1E+03	[mg.kg-1.d-1]	O
Oral NOAEL (mattox)	150	[mg.kg-1.d-1]	S
NOEC via food (mattox)	1.5E+03	[mg.kg-1]	O
Inhalatory NOAEL (mattox)	262	[mg.m-3]	O
Dermal NOAEL (mattox)	150	[mg.kg-1.d-1]	O
Oral NOAEL (devtox)	150	[mg.kg-1.d-1]	S
NOEC via food (devtox)	1.5E+03	[mg.kg-1]	O
Inhalatory NOAEL (devtox)	262	[mg.m-3]	O
Dermal NOAEL (devtox)	150	[mg.kg-1.d-1]	O
Duration of (sub-)chronic oral test	28 days		D
NOEC via food for secondary poisoning	1E+04	[mg.kg-1]	O
PNEC for secondary poisoning of birds and mammals	33.3	[mg.kg-1]	O

Name	Value	Units	Status
ENVIRONMENT - RISK CHARACTERIZATION			
LOCAL [1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
RCR for the local fresh-water compartment	1.7	[-]	O
RCR for the local fresh-water compartment, statistical method	??	[-]	O
RCR for the local marine compartment	17	[-]	O
RCR for the local marine compartment, statistical method	??	[-]	O
RCR for the local fresh-water sediment compartment	17	[-]	O
RCR for the local marine sediment compartment	17	[-]	O
RCR for the local soil compartment	24.3	[-]	O
RCR for the local soil compartment, statistical method	??	[-]	O
RCR for the sewage treatment plant	9.01	[-]	O
RCR for fish-eating birds and mammals (fresh-water)	0.131	[-]	O
RCR for fish-eating birds and mammals (marine)	0.0131	[-]	O
RCR for top predators (marine)	2.62E-03	[-]	O
RCR for worm-eating birds and mammals	0.123	[-]	O
ENVIRONMENT - RISK CHARACTERIZATION			
LOCAL [2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
RCR for the local fresh-water compartment	25.6	[-]	O
RCR for the local fresh-water compartment, statistical method	??	[-]	O
RCR for the local marine compartment	25.7	[-]	O
RCR for the local marine compartment, statistical method	??	[-]	O
RCR for the local fresh-water sediment compartment	25.6	[-]	O
RCR for the local marine sediment compartment	25.7	[-]	O
RCR for the local soil compartment	0.83	[-]	O
RCR for the local soil compartment, statistical method	??	[-]	O
RCR for the sewage treatment plant	13.6	[-]	O
RCR for fish-eating birds and mammals (fresh-water)	0.24	[-]	O
RCR for fish-eating birds and mammals (marine)	0.024	[-]	O
RCR for top predators (marine)	4.8E-03	[-]	O
RCR for worm-eating birds and mammals	2.26E-03	[-]	O
ENVIRONMENT - RISK CHARACTERIZATION			
LOCAL [3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
RCR for the local fresh-water compartment	54.2	[-]	O
RCR for the local fresh-water compartment, statistical method	??	[-]	O
RCR for the local marine compartment	54.2	[-]	O
RCR for the local marine compartment, statistical method	??	[-]	O
RCR for the local fresh-water sediment compartment	54.2	[-]	O
RCR for the local marine sediment compartment	54.2	[-]	O
RCR for the local soil compartment	1.66	[-]	O
RCR for the local soil compartment, statistical method	??	[-]	O
RCR for the sewage treatment plant	28.7	[-]	O
RCR for fish-eating birds and mammals (fresh-water)	0.0693	[-]	O
RCR for fish-eating birds and mammals (marine)	6.94E-03	[-]	O
RCR for top predators (marine)	1.4E-03	[-]	O
RCR for worm-eating birds and mammals	4.27E-03	[-]	O
ENVIRONMENT - RISK CHARACTERIZATION			
REGIONAL			
RCR for the regional fresh-water compartment	7.44E-04	[-]	O
RCR for the regional fresh-water compartment, statistical method	??	[-]	O
RCR for the regional marine compartment	4.54E-03	[-]	O
RCR for the regional marine compartment, statistical method	??	[-]	O
RCR for the regional fresh-water sediment compartment	0.0141	[-]	O
RCR for the regional marine sediment compartment	0.141	[-]	O
RCR for the regional soil compartment	0.0838	[-]	O
RCR for the regional soil compartment, statistical method	??	[-]	O

Name	Value	Units	Status
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
Purification factor for surface water	1	[-]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
CONCENTRATIONS IN INTAKE MEDIA [1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
Local concentration in wet fish	8.71	[mg.kg-1]	O
Local concentration in root tissue of plant	9.94	[mg.kg-1]	O
Local concentration in leaves of plant	2.34	[mg.kg-1]	O
Local concentration in grass (wet weight)	2.32	[mg.kg-1]	O
Local concentration in drinking water	10.6	[mg.l-1]	O
Local concentration in meat (wet weight)	5.88E-04	[mg.kg-1]	O
Local concentration in milk (wet weight)	5.88E-03	[mg.kg-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
DOSES IN INTAKE MEDIA [1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
Daily dose through intake of drinking water	0.303	[mg.kg-1.d-1]	O
Daily dose through intake of fish	0.0143	[mg.kg-1.d-1]	O
Daily dose through intake of leaf crops	0.0401	[mg.kg-1.d-1]	O
Daily dose through intake of root crops	0.0545	[mg.kg-1.d-1]	O
Daily dose through intake of meat	2.53E-06	[mg.kg-1.d-1]	O
Daily dose through intake of milk	4.72E-05	[mg.kg-1.d-1]	O
Daily dose through intake of air	7.98E-09	[mg.kg-1.d-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
FRACTIONS OF TOTAL DOSE [1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
Fraction of total dose through intake of drinking water	0.735	[-]	O
Fraction of total dose through intake of fish	0.0347	[-]	O
Fraction of total dose through intake of leaf crops	0.0973	[-]	O
Fraction of total dose through intake of root crops	0.132	[-]	O
Fraction of total dose through intake of meat	6.14E-06	[-]	O
Fraction of total dose through intake of milk	1.14E-04	[-]	O
Fraction of total dose through intake of air	1.94E-08	[-]	O
Local total daily intake for humans	0.412	[mg.kg-1.d-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
CONCENTRATIONS IN INTAKE MEDIA [2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
Local concentration in wet fish	16	[mg.kg-1]	O
Local concentration in root tissue of plant	0.182	[mg.kg-1]	O
Local concentration in leaves of plant	0.38	[mg.kg-1]	O
Local concentration in grass (wet weight)	0.353	[mg.kg-1]	O
Local concentration in drinking water	11.3	[mg.l-1]	O
Local concentration in meat (wet weight)	5.13E-04	[mg.kg-1]	O
Local concentration in milk (wet weight)	5.13E-03	[mg.kg-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
DOSES IN INTAKE MEDIA [2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
Daily dose through intake of drinking water	0.323	[mg.kg-1.d-1]	O
Daily dose through intake of fish	0.0262	[mg.kg-1.d-1]	O
Daily dose through intake of leaf crops	6.51E-03	[mg.kg-1.d-1]	O
Daily dose through intake of root crops	9.96E-04	[mg.kg-1.d-1]	O
Daily dose through intake of meat	2.21E-06	[mg.kg-1.d-1]	O
Daily dose through intake of milk	4.11E-05	[mg.kg-1.d-1]	O
Daily dose through intake of air	1.59E-04	[mg.kg-1.d-1]	O

Printed on	15-12-2017 17:11:07
Study	Trifluoroacetic acid
Substance	TFA 2100 Plateau, high EC50
Defaults	Standard Euses 2.1
Assessment types	1A, 1B, 2, 3A, 3B
Base set complete	No

Name	Value	Units	Status
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
FRACTIONS OF TOTAL DOSE [2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
Fraction of total dose through intake of drinking water	0.905	[-]	O
Fraction of total dose through intake of fish	0.0735	[-]	O
Fraction of total dose through intake of leaf crops	0.0182	[-]	O
Fraction of total dose through intake of root crops	2.79E-03	[-]	O
Fraction of total dose through intake of meat	6.18E-06	[-]	O
Fraction of total dose through intake of milk	1.15E-04	[-]	O
Fraction of total dose through intake of air	4.45E-04	[-]	O
Local total daily intake for humans	0.357	[mg.kg-1.d-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
CONCENTRATIONS IN INTAKE MEDIA [3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
Local concentration in wet fish	4.62	[mg.kg-1]	O
Local concentration in root tissue of plant	0.343	[mg.kg-1]	O
Local concentration in leaves of plant	0.427	[mg.kg-1]	O
Local concentration in grass (wet weight)	0.371	[mg.kg-1]	O
Local concentration in drinking water	3.27	[mg.l-1]	O
Local concentration in meat (wet weight)	1.63E-04	[mg.kg-1]	O
Local concentration in milk (wet weight)	1.63E-03	[mg.kg-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
DOSES IN INTAKE MEDIA [3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
Daily dose through intake of drinking water	0.0935	[mg.kg-1.d-1]	O
Daily dose through intake of fish	7.59E-03	[mg.kg-1.d-1]	O
Daily dose through intake of leaf crops	7.32E-03	[mg.kg-1.d-1]	O
Daily dose through intake of root crops	1.88E-03	[mg.kg-1.d-1]	O
Daily dose through intake of meat	7.01E-07	[mg.kg-1.d-1]	O
Daily dose through intake of milk	1.31E-05	[mg.kg-1.d-1]	O
Daily dose through intake of air	1.63E-04	[mg.kg-1.d-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL SCALE			
FRACTIONS OF TOTAL DOSE [3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
Fraction of total dose through intake of drinking water	0.846	[-]	O
Fraction of total dose through intake of fish	0.0687	[-]	O
Fraction of total dose through intake of leaf crops	0.0663	[-]	O
Fraction of total dose through intake of root crops	0.0171	[-]	O
Fraction of total dose through intake of meat	6.34E-06	[-]	O
Fraction of total dose through intake of milk	1.18E-04	[-]	O
Fraction of total dose through intake of air	1.48E-03	[-]	O
Local total daily intake for humans	0.11	[mg.kg-1.d-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
REGIONAL SCALE			
CONCENTRATIONS IN INTAKE MEDIA			
Regional concentration in wet fish	4.63E-04	[mg.kg-1]	O
Regional concentration in root tissue of plant	3.08E-04	[mg.kg-1]	O
Regional concentration in leaves of plant	7.48E-05	[mg.kg-1]	O
Regional concentration in grass (wet weight)	7.48E-05	[mg.kg-1]	O
Regional concentration in drinking water	1.23E-04	[mg.l-1]	S
Regional concentration in meat (wet weight)	1.12E-08	[mg.kg-1]	O
Regional concentration in milk (wet weight)	1.12E-07	[mg.kg-1]	O

Name	Value	Units	Status
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
REGIONAL SCALE			
DOSES IN INTAKE MEDIA			
Daily dose through intake of drinking water	3.51E-06	[mg.kg-1.d-1]	O
Daily dose through intake of fish	7.61E-07	[mg.kg-1.d-1]	O
Daily dose through intake of leaf crops	1.28E-06	[mg.kg-1.d-1]	O
Daily dose through intake of root crops	1.69E-06	[mg.kg-1.d-1]	O
Daily dose through intake of meat	4.83E-11	[mg.kg-1.d-1]	O
Daily dose through intake of milk	9.01E-10	[mg.kg-1.d-1]	O
Daily dose through intake of air	1.17E-09	[mg.kg-1.d-1]	O
HUMAN HEALTH - EXPOSURE ASSESSMENT			
HUMANS EXPOSED VIA THE ENVIRONMENT			
REGIONAL SCALE			
FRACTIONS OF TOTAL DOSE			
Fraction of total dose through intake of drinking water	0.485	[-]	O
Fraction of total dose through intake of fish	0.105	[-]	O
Fraction of total dose through intake of leaf crops	0.177	[-]	O
Fraction of total dose through intake of root crops	0.233	[-]	O
Fraction of total dose through intake of meat	6.67E-06	[-]	O
Fraction of total dose through intake of milk	1.24E-04	[-]	O
Fraction of total dose through intake of air	1.62E-04	[-]	O
Regional total daily intake for humans	7.25E-06	[mg.kg-1.d-1]	O

Name	Value	Units	Status
HUMAN HEALTH - RISK CHARACTERIZATION			
CURRENT CLASSIFICATION			
Corrosive (C, R34 or R35)	Yes		S
Irritating to skin (Xi, R38)	No		D
Irritating to eyes (Xi, R36)	No		D
Risk of serious damage to eyes (Xi, R41)	No		D
Irritating to respiratory system (Xi, R37)	No		D
May cause sensitisation by inhalation (Xn, R42)	No		D
May cause sensitisation by skin contact (Xi, R43)	No		D
May cause cancer (T, R45)	No		D
May cause cancer by inhalation (T, R49)	No		D
Possible risk of irreversible effects (Xn, R40)	No		D
HUMAN HEALTH - RISK CHARACTERIZATION			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL [1 "CHEMICAL PRODUCTION", IC=3/UC=29][PRODUCTION]			
MOS, local, inhalatory (repdose)	6.26E+10	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (repdose)	6.26E+10	[-]	O
MOS, local, total exposure (repdose)	2.43E+03	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (repdose)	2.43E+03	[-]	O
MOS, local, inhalatory (fert)	6.26E+10	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (fert)	6.26E+10	[-]	O
MOS, local, total exposure (fert)	2.43E+03	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (fert)	2.43E+03	[-]	O
MOS, local, inhalatory (mattox)	9.4E+09	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (mattox)	9.4E+09	[-]	O
MOS, local, total exposure (mattox)	364	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (mattox)	364	[-]	O
MOS, local, inhalatory (devtox)	9.4E+09	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (devtox)	9.4E+09	[-]	O
MOS, local, total exposure (devtox)	364	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (devtox)	364	[-]	O
HUMAN HEALTH - RISK CHARACTERIZATION			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL [2 "PERSONAL DOMESTIC HEATING/COOLING", IC=5/UC=29][PRIVATE USE]			
MOS, local, inhalatory (repdose)	3.15E+06	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (repdose)	3.15E+06	[-]	O
MOS, local, total exposure (repdose)	2.8E+03	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (repdose)	2.8E+03	[-]	O
MOS, local, inhalatory (fert)	3.15E+06	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (fert)	3.15E+06	[-]	O
MOS, local, total exposure (fert)	2.8E+03	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (fert)	2.8E+03	[-]	O
MOS, local, inhalatory (mattox)	4.72E+05	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (mattox)	4.72E+05	[-]	O
MOS, local, total exposure (mattox)	420	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (mattox)	420	[-]	O
MOS, local, inhalatory (devtox)	4.72E+05	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (devtox)	4.72E+05	[-]	O
MOS, local, total exposure (devtox)	420	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (devtox)	420	[-]	O

Name	Value	Units	Status
HUMAN HEALTH - RISK CHARACTERIZATION			
HUMANS EXPOSED VIA THE ENVIRONMENT			
LOCAL [3 "LIGHT INDUSTRIAL USE HEATING.COOLING", IC=6/UC=29][INDUSTRIAL USE]			
MOS, local, inhalatory (repdose)	3.06E+06	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (repdose)	3.06E+06	[-]	O
MOS, local, total exposure (repdose)	9.05E+03	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (repdose)	9.05E+03	[-]	O
MOS, local, inhalatory (fert)	3.06E+06	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (fert)	3.06E+06	[-]	O
MOS, local, total exposure (fert)	9.05E+03	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (fert)	9.05E+03	[-]	O
MOS, local, inhalatory (mattox)	4.6E+05	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (mattox)	4.6E+05	[-]	O
MOS, local, total exposure (mattox)	1.36E+03	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (mattox)	1.36E+03	[-]	O
MOS, local, inhalatory (devtox)	4.6E+05	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (devtox)	4.6E+05	[-]	O
MOS, local, total exposure (devtox)	1.36E+03	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (devtox)	1.36E+03	[-]	O
HUMAN HEALTH - RISK CHARACTERIZATION			
HUMANS EXPOSED VIA THE ENVIRONMENT			
REGIONAL			
MOS, regional, inhalatory (repdose)	4.27E+11	[-]	O
Ratio MOS/Ref-MOS, regional, inhalatory (repdose)	4.27E+11	[-]	O
MOS, regional, total exposure (repdose)	1.38E+08	[-]	O
Ratio MOS/Ref-MOS, regional, total exposure (repdose)	1.38E+08	[-]	O
MOS, regional, inhalatory (fert)	4.27E+11	[-]	O
Ratio MOS/Ref-MOS, regional, inhalatory (fert)	4.27E+11	[-]	O
MOS, regional, total exposure (fert)	1.38E+08	[-]	O
Ratio MOS/Ref-MOS, regional, total exposure (fert)	1.38E+08	[-]	O
MOS, regional, inhalatory (mattox)	6.4E+10	[-]	O
Ratio MOS/Ref-MOS, regional, inhalatory (mattox)	6.4E+10	[-]	O
MOS, regional, total exposure (mattox)	2.07E+07	[-]	O
Ratio MOS/Ref-MOS, regional, total exposure (mattox)	2.07E+07	[-]	O
MOS, regional, inhalatory (devtox)	6.4E+10	[-]	O
Ratio MOS/Ref-MOS, regional, inhalatory (devtox)	6.4E+10	[-]	O
MOS, regional, total exposure (devtox)	2.07E+07	[-]	O
Ratio MOS/Ref-MOS, regional, total exposure (devtox)	2.07E+07	[-]	O

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