

S1 | Free aqueous concentrations for human loss of consciousness and rodent loss of righting reflex*

Molecular Weight	Mouse or rat LORR [‡]	Human loss of consciousness [§]	Ostwald coefficient at 37°C (for gas/buffer)	Protein binding or partition data	Rodent concentration for LORR (mM)	Human concentration for LOC (mM)
Nitrous oxide (N₂O; N#[N+][O-])						
44.01	1.18 atm ¹	0.650 atm ²	0.47 ³ ×0.94 ¹⁴		20.5	11.3
Cyclopropane (C₃H₆; C1CC1)						
42.08	0.151 atm ¹	0.07 atm ^{5,6}	0.21 ³ ×0.94 ¹⁴		1.17	0.54
Xenon (Xe; [Xe])						
131.29	0.95 atm ²	0.33 atm ⁷	0.085 ¹² ×0.94 ¹⁴		2.98	1.04
Desflurane (C₃H₂F₆O; C(C(F)(F)F)(OC(F)F)F)						
168.04	0.0733 atm ⁹	0.0251 atm ²	0.225 ¹⁰		0.648	0.222
Sevoflurane (C₄H₃F₇O; C(OC(C(F)(F)F)C(F)(F)F)F)						
200.05	0.020 atm ^{9,11}	0.00648 atm ²	0.370 ¹²		0.291	0.094
Isoflurane (C₃H₂ClF₅O; C(C(F)(F)F)(OC(F)F)Cl)						
184.49	0.0060 atm ^{11,13}	0.00414 atm ²	0.534 ⁸		0.126	0.087
Halothane (C₂HBrClF₃; C(C(F)(F)F)(Cl)Br)						
197.38	0.0075 atm ^{9,11,13}	0.0041 atm ²	0.659 ⁸		0.194	0.106
Thiopental (C₁₁H₁₈N₂O₂S; CCCC(C)C1(C(=O)NC(=S)NC1=O)CC)						
242.34	15.9 mg/ml in plasma ¹⁴	15.6 mg/ml in serum ¹⁵		85% protein binding ¹⁶	0.0099	0.0097
Propofol (C₁₂H₁₈O; CC(C)C1=C(C(=CC=C1)C(C)C)O)						
178.27	3.8 mg/ml in blood ¹⁷	3.0 mg/ml in blood ^{18,19}		97.8% protein binding ²⁰	0.00047	0.00037
Etomidate (C₁₄H₁₆N₂O₂; CCOC(=O)C1=CN=CN1C(C)C2=CC=CC=C2)						
244.29	0.44 mg/ml in plasma ²¹	0.25 mg/ml plasma ^{22–24}		Plasma/buffer partition coefficient 4.3 ²⁵	0.0018	0.001

*Compound followed by molecular formula and SMILES notation in brackets. †No distinction is made between provoked, and unprovoked, loss of righting reflex. ‡Failure to respond to a verbal command. ||In some cases, Ostwald coefficients have been calculated from literature values for Bunsen coefficients using the relationship: Ostwald coefficient = Bunsen coefficient × 1.13546. ††This reduction of 6% accounts for the reduced solubility of anaesthetics in physiological saline solution compared to pure water according to reference 4.

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