

Tryptophol

Other names:	1H-Indole-3-ethanol 1H-Indolyl-3-ethanol 2-(1H-indol-3-yl)ethanol 2-(3-indolyl)ethanol 3-(2-hydroxyethyl)-1H-indole 3-(2-hydroxyethyl)indole 3-(«beta»-Hydroxyethyl)indole 3-Indoleethanol 3-Indolyethanol Ethanol, 2-indol-3-yl- Ethanol, 3-indolyl- IEA Indole-3-ethanol Indoleethanol NSC 3884 dl-Tryptophanol «beta»-(3-Indole)ethanol «beta»-indol-3-ylethanol
Inchi:	InChI=1S/C10H11NO/c12-6-5-8-7-11-10-4-2-1-3-9(8)10/h1-4,7,11-12H,5-6H2
InchiKey:	MBBOMCVGYCRMEA-UHFFFAOYSA-N
Formula:	C10H11NO
SMILES:	OCCc1c[nH]c2ccccc12
Mol. weight [g/mol]:	161.20
CAS:	526-55-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.56		Crippen Method
logp	1.221		Crippen Method
mcpvol	128.690	ml/mol	McGowan Method
rinpol	1750.00		NIST Webbook
rinpol	1787.70		NIST Webbook
rinpol	1750.00		NIST Webbook
ripol	2882.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	119.80	kJ/mol	298.15	Calorimetric and computational study of (1H-Indol-n-yl)methanol and 2-(1H-Indol-n-yl)ethanol (n=2, 3)

Sources

Calorimetric and computational study of (1H-Indol-n-yl)methanol and 2-(1H-Indol-n-yl)ethanol (n=2, 3):	https://www.doi.org/10.1016/j.tca.2019.01.021
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C526556&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/23-713-4/Tryptophol.pdf>

Generated by Cheméo on 2024-04-26 09:25:42.652144197 +0000 UTC m=+16412791.572721508.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.