

Tetrahydrorhombifoline

Inchi: InChI=1S/C15H24N2O/c1-2-3-7-16-9-12-8-13(11-16)14-5-4-6-15(18)17(14)10-12/h2,12-
InchiKey: OKTIETCHYDTVGN-UHFFFAOYSA-N
Formula: C15H24N2O
SMILES: C=CCCN1CC2CC(C1)C1CCCC(=O)N1C2
Mol. weight [g/mol]: 248.36
CAS: 3382-84-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.18		Crippen Method
logp	1.895		Crippen Method
mcvol	206.860	ml/mol	McGowan Method
rinpol	2050.00		NIST Webbook
rinpol	2080.00		NIST Webbook
rinpol	2050.00		NIST Webbook
rinpol	2050.00		NIST Webbook
rinpol	2050.00		NIST Webbook
rinpol	2050.00		NIST Webbook
rinpol	2040.00		NIST Webbook
rinpol	2050.00		NIST Webbook
rinpol	2050.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C3382841&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcpol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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