

13-Methoxylupanine

Inchi: InChI=1S/C16H26N2O2/c1-20-13-5-6-14-12-7-11(8-17(14)10-13)15-3-2-4-16(19)18(15)9
InchiKey: YEDHYJZNGSWGER-UHFFFAOYSA-N
Formula: C16H26N2O2
SMILES: COC1CCC2C3CC(CN2C1)C1CCCC(=O)N1C3
Mol. weight [g/mol]: 278.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.95		Crippen Method
logp	1.497		Crippen Method
mcvol	220.260	ml/mol	McGowan Method
rinpole	2370.00		NIST Webbook
rinpole	2370.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R263960&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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<https://www.chemeo.com/cid/13-148-3/13-Methoxylupanine.pdf>

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