

6-N orcarnegine

Inchi: InChI=1S/C12H17NO2/c1-8-10-7-12(15-3)11(14)6-9(10)4-5-13(8)2/h6-8,14H,4-5H2,1-3H
InchiKey: BQWXVEGUQMSXOH-UHFFFAOYSA-N
Formula: C12H17NO2
SMILES: COc1cc2c(cc1O)CCN(C)C2C
Mol. weight [g/mol]: 207.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.09		Crippen Method
logp	1.950		Crippen Method
mcvol	167.040	ml/mol	McGowan Method
rinpol	1715.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R299553&Units=SI>

Legend

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

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<https://www.chemeo.com/cid/35-644-8/6-N-orcarnegine.pdf>

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