

7-N orcarnegine

Inchi: InChI=1S/C12H17NO2/c1-8-10-7-11(14)12(15-3)6-9(10)4-5-13(8)2/h6-8,14H,4-5H2,1-3H3
InchiKey: QFSVLNAGJRAZFV-UHFFFAOYSA-N
Formula: C12H17NO2
SMILES: COc1cc2c(cc1O)C(C)N(C)CC2
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
rinpol	1715.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R299593&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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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