

Creatonotine

Inchi: InChI=1S/C14H23NO4/c1-3-9(2)13(17)14(18)19-8-10-4-6-15-7-5-11(16)12(10)15/h4,9,11,12,13,14,15,16,17,18,19
InchiKey: GHJLDQVAJMAZBR-LPTSXCQYSA-N
Formula: C14H23NO4
SMILES: CCC(C)C(O)C(=O)OCC1=CCN2CCC(O)C12
Mol. weight [g/mol]: 269.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.38		Crippen Method
logp	0.312		Crippen Method
mcvol	211.260	ml/mol	McGowan Method
rinpol	1985.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R178397&Units=SI>
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>

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/50-670-2/Creatonotine.pdf>

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