

Concneorine

Inchi: InChI=1S/C16H21NO4/c1-17-11-4-5-12(17)9-13(8-11)21-16(19)10-3-6-14(18)15(7-10)20
InchiKey: OZKTVDIYALBSMA-CLLJXQQHSA-N
Formula: C16H21NO4
SMILES: COc1cc(C(=O)OC2CC3CCCC(C2)N3C)ccc1O
Mol. weight [g/mol]: 291.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.01		Crippen Method
logp	2.183		Crippen Method
mcvol	219.980	ml/mol	McGowan Method
rinpol	2365.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R510008&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

Latest version available from:

<https://www.chemeo.com/cid/17-580-9/Concneorine.pdf>

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