

Ipanguline D7

Inchi: InChI=1S/C16H21NO3/c18-14-7-9-17-8-6-13(16(14)17)11-20-15(19)10-12-4-2-1-3-5-12/
InchiKey: JXZUYJXDSHOAGV-ADTLFGHVSA-N
Formula: C16H21NO3
SMILES: O=C(Cc1ccccc1)OCC1CCN2CCC(O)C12
Mol. weight [g/mol]: 275.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.09		Crippen Method
logp	1.227		Crippen Method
mcvol	214.110	ml/mol	McGowan Method
rinpol	2212.00		NIST Webbook
rinpol	2212.00		NIST Webbook
rinpol	2212.00		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=R395047&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/51-780-9/lpanguline-D7.pdf>

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