

Dropropizine

Inchi: InChI=1S/C13H20N2O2/c16-11-13(17)10-14-6-8-15(9-7-14)12-4-2-1-3-5-12/h1-5,13,16-17
InchiKey: PTVWPYVOOKLBCG-UHFFFAOYSA-N
Formula: C13H20N2O2
SMILES: OCC(O)CN1CCN(c2ccccc2)CC1
Mol. weight [g/mol]: 236.31
CAS: 17692-31-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.58		Crippen Method
logp	0.162		Crippen Method
mcvol	191.110	ml/mol	McGowan Method
rinpola	2112.00		NIST Webbook
rinpola	2112.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C17692318&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
rinpola: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/119-047-8/Dropropizine.pdf>

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