

Ipanguline D12

Inchi: InChI=1S/C13H23NO5/c1-8(16)13(2,18)12(17)19-10-4-6-14-5-3-9(7-15)11(10)14/h8-11,13-15,17-18,20-21/t12,14,16,18,20
InchiKey: JUKASHKBUGPLHM-LFEBVRLFSA-N
Formula: C13H23NO5
SMILES: CC(O)C(C)(O)C(=O)OC1CCN2CCC(CO)C12
Mol. weight [g/mol]: 273.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.48		Crippen Method
logp	-0.883		Crippen Method
mcvol	207.340	ml/mol	McGowan Method
rinpol	2125.00		NIST Webbook
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rinpol	2125.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R394960&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/13-221-1/ipanguline-D12.pdf>

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