

Ipanguline D10

Inchi: InChI=1S/C18H31NO6/c1-5-11(2)16(21)25-12(3)18(4,23)17(22)24-10-13-6-8-19-9-7-14(15)
InchiKey: QGMFKSHYVNTQIZ-FCQBRQFGSA-N
Formula: C18H31NO6
SMILES: CCC(C)C(=O)OC(C)C(C)(O)C(=O)OCC1CCN2CCC(O)C12
Mol. weight [g/mol]: 357.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.93		Crippen Method
logp	0.714		Crippen Method
mcvol	279.360	ml/mol	McGowan Method
rinpol	2349.00		NIST Webbook
rinpol	2327.00		NIST Webbook
rinpol	2327.00		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=R394955&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/13-426-4/lpanguline-D10.pdf>

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