Ipanguline D1

Inchi: InChI=1S/C12H21NO3/c1-2-3-11(15)16-8-9-4-6-13-7-5-10(14)12(9)13/h9-10,12,14H,2-8
InchiKey: XHOXLWVKPKHLFN-HVFQMFNGSA-N
Formula: C12H21NO3
SMILES: CCCC(=O)OCC1CCN2CCC(O)C12
Mol. weight [g/mol]: 227.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.31		Crippen Method
logp	0.785		Crippen Method
mcvol	181.510	ml/mol	McGowan Method
rinpol	1703.00		NIST Webbook
rinpol	1703.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R394940&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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