Ipanguline D3

Inchi: InChI=1S/C13H23NO5/c1-8(15)13(2,18)12(17)19-7-9-3-5-14-6-4-10(16)11(9)14/h8-11,15
InchiKey: GWTMMYYKPSYPDW-LFEBVRLFSA-N
Formula: C13H23NO5
SMILES: CC(O)C(C)(O)C(=O)OCC1CCN2CCC(O)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	2037.00		NIST Webbook
rinpol	2037.00		NIST Webbook
rinpol	2037.00		NIST Webbook

Sources

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=R395012&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices