Ipanguline D5

Inchi: InChI=1S/C15H25NO6/c1-9(22-10(2)17)15(3,20)14(19)21-8-11-4-6-16-7-5-12(18)13(11)1
InchiKey: NWXBPCGWPSVFTO-CVARFHGKSA-N
Formula: C15H25NO6
SMILES: CC(=O)OC(C)C(C)(O)C(=O)OCC1CCN2CCC(O)C12
Mol. weight [g/mol]: 315.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.92		Crippen Method
logp	-0.313		Crippen Method
mcvol	237.090	ml/mol	McGowan Method
rinpol	2157.00		NIST Webbook
rinpol	2157.00		NIST Webbook
rinpol	2157.00		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=R395032&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