Isoipanguline D9

Inchi: InChI=1S/C17H27NO7/c1-10(24-11(2)19)17(4,25-12(3)20)16(22)23-9-13-5-7-18-8-6-14(
InchiKey: ZFNBQBCMFVRFDH-BQGRYJDESA-N
Formula: C17H27NO7
SMILES: CC(=O)OC(C)C(C)(OC(C)=O)C(=O)OCC1CCN2CCC(O)C12
Mol. weight [g/mol]: 357.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.35		Crippen Method
logp	0.258		Crippen Method
mcvol	266.840	ml/mol	McGowan Method
rinpol	2246.00		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=R414252&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