Ipanguline D18

Inchi:	InChI=1S/C18H29NO6/c1-5-11(2)16(21)25-12(3)18(4,23)17(22)24-10-13-6-8-19-9-7-14(
InchiKey:	QZDRHOHMWBXGER-LXQJWIEQSA-N
Formula:	C18H29NO6
SMILES:	CC=C(C)C(=O)OC(C)C(C)(O)C(=O)OCC1CCN2CCC(O)C12
Mol. weight [g/mol]:	355.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.03		Crippen Method
logp	0.634		Crippen Method
mcvol	275.060	ml/mol	McGowan Method
rinpol	2480.00		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=R414232&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

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