Pumiline A

Inchi: InChI=1S/C18H25NO6/c1-10(2)13-15(20)25-12-5-7-19-6-4-11(14(12)19)8-23-16(21)17(3
InchiKey: RTWHYIZIQSNTMZ-HWQRRKCRSA-N
Formula: C18H25NO6
SMILES: CC(C)C1C(=O)OC2CCN3CC=C(COC(=O)C(C)(O)C14CO4)C23
Mol. weight [g/mol]: 351.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.40		Crippen Method
logp	0.261		Crippen Method
mcvol	253.340	ml/mol	McGowan Method
rinpol	2473.00		NIST Webbook
rinpol	2473.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R590331&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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