Jacoline

Inchi: InChI=1S/C18H27NO7/c1-10-8-18(24,11(2)20)16(22)26-13-5-7-19-6-4-12(14(13)19)9-25
InchiKey: FMWJEBGSMAOQNN-UHFFFAOYSA-N
Formula: C18H27NO7
SMILES: CC1CC(O)(C(C)O)C(=O)OC2CCN3CC=C(COC(=O)C1(C)O)C23
Mol. weight [g/mol]: 369.41
CAS: 480-76-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.30		Crippen Method
logp	-0.642		Crippen Method
mcvol	270.070	ml/mol	McGowan Method
rinpol	2508.00		NIST Webbook
rinpol	2485.00		NIST Webbook
rinpol	2488.00		NIST Webbook
rinpol	2535.00		NIST Webbook
rinpol	2488.00		NIST Webbook
rinpol	2488.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C480762&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