O-Crotaverrine

Inchi: InChI=1S/C19H27NO6/c1-5-13-10-12(2)19(3,24)18(23)25-11-14-6-8-20(4)9-7-15(16(14)2
InchiKey: HPDHKHMHQGCNPE-AGYIUGPWSA-N
Formula: C19H27NO6
SMILES: CC=C1CC(C)C(C)(O)C(=O)OCC2=CCN(C)CCC(OC1=O)C2=O
Mol. weight [g/mol]: 365.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.09		Crippen Method
logp	1.010		Crippen Method
mcvol	280.550	ml/mol	McGowan Method
rinpol	2710.00		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=R590326&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