Methylmonocrotaline

Inchi: InChI=1S/C17H25NO6/c1-15(2)13(19)24-11-6-8-18-7-5-10(12(11)18)9-23-14(20)16(3,21
InchiKey: NQHCYMOPENHUTC-XUTRHLIJSA-N
Formula: C17H25NO6
SMILES: CC1(C)C(=O)OC2CCN3CC=C(COC(=O)C(C)(O)C1(C)O)C23
Mol. weight [g/mol]: 339.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.50		Crippen Method
logp	-0.002		Crippen Method
mcvol	250.110	ml/mol	McGowan Method
rinpol	2351.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R405357&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices