Renardine

Other names:	Renardine (neutral) Senecionanium, 8,12-dihydroxy-4-methyl-11,16-dioxo- Senkarkane Senkirkine Senkirkine (neutral) 2,12-Dihydroxy-4-methyl-11,16-dioxosenecionanium 4,8-Secosenecionan-8,11,16-trione, 12-hydroxy-4-methyl- trans-15-Ethylidene-12-«beta»-hydroxy-4,12-«alpha»,13-«beta»-trimethyl 8-oxo-4,8 secosenec-1-enine
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-GFIWHYBVSA-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
CAS:	2318-18-5

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	2540.00		NIST Webbook
rinpol	2530.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2318185&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