

Senecionine

Other names:	Aureine Senecionan-11,16-dione, 12-hydroxy- Senecionin 12-Hydroxysenecionan-11,16-dione Sencionine [1,6]Dioxacyclododecino[2,3,4-gh]pyrrolizine-2,7-dione, 3-ethylidene-3,4,5,6,9,11,13,14,14a,14b-decahydro-6-hydroxy-5,6-dimethyl-, 12-hydroxysenecionane-11,16-dione (3Z,5R,6R,14aR,14bR)
Inchi:	InChI=1S/C18H25NO5/c1-4-12-9-11(2)18(3,22)17(21)23-10-13-5-7-19-8-6-14(15(13)19)
InchiKey:	HKODIGSRFALUTA-ZWGWPGHTSA-N
Formula:	C18H25NO5
SMILES:	CC=C1CC(C)C(C)(O)C(=O)OCC2=CCN3CCC(OC1=O)C23
Mol. weight [g/mol]:	335.39
CAS:	130-01-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.40		Crippen Method
logp	1.193		Crippen Method
mvol	254.030	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C130018&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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