Seneciphylline

Other names:	Jacodine
	NSC 30622
	Pyrrolizine-2,7-dione, 3-ethylidene-3,4,5,6,9,11,13,14,14a,14b-decahydro-6-hydroxy-6-methyl-5-methylene(1,6)
	Senecionan-11,16-dione, 13,19-didehydro-12-hydroxy-
	Seneciphyllin
	[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-6-methyl-5-methylene-, (3Z,6R,14aR,14bR)-
	13,19-Didehydro-12-hydroxy senecionane-11,16-dione
Inchi:	InChI=1S/C18H23NO5/c1-4-12-9-11(2)18(3,22)17(21)23-10-13-5-7-19-8-6-14(15(13)19)2
InchiKey:	FCEVNJIUIMLVML-UUILKARUSA-N
Formula:	C18H23NO5
SMILES:	C=C1CC(=CC)C(=O)OC2CCN3CC=C(COC(=O)C1(C)O)C23
Mol. weight [g/mol]:	333.38
CAS:	480-81-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.50		Crippen Method
logp	1.113		Crippen Method
mcvol	249.730	ml/mol	McGowan Method
rinpol	2303.00		NIST Webbook
rinpol	2306.00		NIST Webbook
rinpol	2320.00		NIST Webbook
rinpol	2360.00		NIST Webbook
rinpol	2327.00		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=C480819&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