(Z)-Erucifoline

Inchi: InChI=1S/C18H23NO5/c1-4-11-9-17(2)18(3,24-17)16(21)22-10-12-5-7-19-8-6-13(14(12)1
InchiKey: XYLHTQLSMWVEML-LCLHOKOMSA-N
Formula: C18H23NO5
SMILES: CC=C1CC2(C)OC2(C)C(=O)OCC2=CCN3CCC(OC1=O)C23
Mol. weight [g/mol]: 333.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.47		Crippen Method
logp	1.353		Crippen Method
mcvol	243.170	ml/mol	McGowan Method
rinpol	2542.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R572784&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