

Erucifoline (E)

Inchi: InChI=1S/C18H23NO6/c1-3-11-8-18(10-20)17(2,25-18)16(22)23-9-12-4-6-19-7-5-13(14)
InchiKey: NOQVBHOUTTZGE-FFIQDWLQSA-N
Formula: C18H23NO6
SMILES: CC=C1CC2(CO)OC2(C)C(=O)OCC2=CCN3CCC(OC1=O)C23
Mol. weight [g/mol]: 349.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.74		Crippen Method
logp	0.326		Crippen Method
mcvol	249.040	ml/mol	McGowan Method
rinpol	2478.00		NIST Webbook
rinpol	2560.00		NIST Webbook
rinpol	2478.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R178164&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

Latest version available from:

<https://www.chemeo.com/cid/53-960-7/Erucifoline-E.pdf>

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