2-O-acetyl-8,12-epoxygermacra-1(10),4,7,11-tetrae
isomer I

Inchi: InChI=1S/C17H22O3/c1-11-5-6-16-13(3)10-19-17(16)9-12(2)8-15(7-11)20-14(4)18/h5,8,
InchiKey: VIAGREYUICSQGX-SSQAHJBYSA-N
Formula: C17H22O3
SMILES: CC(=O)OC1C=C(C)Cc2occ(C)c2CC=C(C)C1
Mol. weight [g/mol]: 274.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.21		Crippen Method
logp	3.901		Crippen Method
mcvol	224.780	ml/mol	McGowan Method
rinpol	1792.00		NIST Webbook

Sources

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=R337234&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices