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

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