

15,16-Epoxyabda-13(16),14-dien-8 «alpha»-ol

Inchi:	InChI=1S/C20H32O2/c1-18(2)10-5-11-19(3)16(18)8-12-20(4,21)17(19)7-6-15-9-13-22-14
InchiKey:	KAFYUFLRNOJDNU-AJZSKMSESA-N
Formula:	C20H32O2
SMILES:	CC1(C)CCCC2(C)C1CCC(C)(O)C2CCc1ccoc1
Mol. weight [g/mol]:	304.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.07		Crippen Method
logp	5.206		Crippen Method
mcvol	263.220	ml/mol	McGowan Method
rinpol	2211.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R432785&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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