

epi-Curzerenone

Inchi: InChI=1S/C15H18O2/c1-6-15(5)7-11-12(10(4)8-17-11)14(16)13(15)9(2)3/h6,8,13H,1-2,7
InchiKey: ZVMJXSJCBLRAPD-UHFFFAOYSA-N
Formula: C15H18O2
SMILES: C=CC1(C)Cc2occ(C)c2C(=O)C1C(=C)C
Mol. weight [g/mol]: 230.30
CAS: 20085-85-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.77		Crippen Method
logp	3.711		Crippen Method
mcvol	190.730	ml/mol	McGowan Method
rinpol	1584.00		NIST Webbook
rinpol	1601.90		NIST Webbook
rinpol	1584.00		NIST Webbook
rinpol	1623.20		NIST Webbook
rinpol	1623.20		NIST Webbook
ripol	2219.00		NIST Webbook
ripol	2219.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C20085852&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
ripol: Polar retention indices

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