Curzerenone

Inchi: InChI=1S/C15H20O2/c1-6-15(5)7-11-12(10(4)8-17-11)14(16)13(15)9(2)3/h8,13H,2,6-7H2
InchiKey: KTDQZLJOUMVWTK-UKRRQHHQSA-N
Formula: C15H18O2
SMILES: C=C(C)C1C(=O)c2c(C)coc2CC1(C)CC
Mol. weight [g/mol]: 230.30
CAS: 20493-56-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.92		Crippen Method
logp	3.935		Crippen Method
mcvol	195.030	ml/mol	McGowan Method
rinpol	1574.00		NIST Webbook
rinpol	1576.00		NIST Webbook
rinpol	1595.50		NIST Webbook
rinpol	1609.60		NIST Webbook
rinpol	1590.00		NIST Webbook
rinpol	1568.00		NIST Webbook
rinpol	1599.00		NIST Webbook
rinpol	1610.00		NIST Webbook
ripol	2278.00		NIST Webbook
ripol	2240.00		NIST Webbook
ripol	2240.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20493565&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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