Zederone

Inchi: InChI=1S/C15H18O3/c1-9-5-4-6-15(3)14(18-15)13(16)12-10(2)8-17-11(12)7-9/h5,8,14H,
InchiKey: CVIVANCKIBYAOP-WEVVVXLNSA-N
Formula: C15H18O3
SMILES: CC1=CCCC2(C)OC2C(=O)c2c(C)coc2C1
Mol. weight [g/mol]: 246.30
CAS: 7727-79-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.61		Crippen Method
logp	3.211		Crippen Method
mcvol	190.040	ml/mol	McGowan Method
rinpol	2009.70		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7727799&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.