Chalepensin

Inchi: InChI=1S/C16H14O3/c1-4-16(2,3)12-8-11-7-10-5-6-18-13(10)9-14(11)19-15(12)17/h4-9H
InchiKey: FYCCCUNGXGKNJV-UHFFFAOYSA-N
Formula: C16H14O3
SMILES: C=CC(C)(C)c1cc2cc3ccoc3cc2oc1=O
Mol. weight [g/mol]: 254.28
CAS: 13164-03-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-13.56		Crippen Method
logp	4.003		Crippen Method
mcvol	191.230	ml/mol	McGowan Method
rinpol	2205.60		NIST Webbook
rinpol	2205.60		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C13164039&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices