Chalepin

Inchi: InChI=1S/C19H22O4/c1-6-18(2,3)13-8-11-7-12-9-16(19(4,5)21)22-14(12)10-15(11)23-17
InchiKey: JCDLLLXYAICSQV-UHFFFAOYSA-N
Formula: C19H22O4
SMILES: C=CC(C)(C)c1cc2cc3c(cc2oc1=O)OC(C(C)(C)O)C3
Mol. weight [g/mol]: 314.38
CAS: 13164-04-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.16		Crippen Method
logp	3.331		Crippen Method
mcvol	243.670	ml/mol	McGowan Method
rinpol	2688.30		NIST Webbook
rinpol	2688.30		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=C13164040&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