

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:	<chem>C=CC(C)(C)c1cc2cc3c(cc2oc1=O)OC(C(C)(C)O)C3</chem>
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
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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

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