Epoxyaurapten

Inchi: InChI=1S/C19H22O4/c1-13(4-8-17-19(2,3)23-17)10-11-21-15-7-5-14-6-9-18(20)22-16(14
InchiKey: KJDXYWIMMJVFLH-JLHYYAGUSA-N
Formula: C19H22O4
SMILES: CC(=CCOc1ccc2ccc(=O)oc2c1)CCC1OC1(C)C
Mol. weight [g/mol]: 314.38
CAS: 36414-00-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.38		Crippen Method
logp	4.076		Crippen Method
mcvol	243.670	ml/mol	McGowan Method
rinpol	2776.40		NIST Webbook
rinpol	2776.40		NIST Webbook
rinpol	2772.00		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=C36414003&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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