

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

Latest version available from:

<https://www.cheméo.com/cid/91-946-1/Epoxyaurapten.pdf>

Generated by Cheméo on 2024-04-25 20:07:46.463827942 +0000 UTC m=+16364915.384405254.

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