

(.+/-.)-Marmesin

Inchi: InChI=1S/C14H14O4/c1-14(2,16)12-6-9-5-8-3-4-13(15)18-10(8)7-11(9)17-12/h3-5,7,12,14
InchiKey: FWYSBEAFFPBAQU-UHFFFAOYSA-N
Formula: C14H14O4
SMILES: CC(C)(O)C1Cc2cc3ccc(=O)oc3cc2O1
Mol. weight [g/mol]: 246.26
CAS: 13710-70-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.57		Crippen Method
logp	1.867		Crippen Method
mcvol	177.520	ml/mol	McGowan Method
rinpol	2341.00		NIST Webbook
rinpol	2341.00		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=C13710708&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.chemeo.com/cid/121-505-6/Marmesin.pdf>

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