7H-Furo[3,2-g][1]benzopyran-7-one, 2,3-dihydro-2-(1-hydroxy-1-methylethyl)-, (S)-

Other names: 7H-Furo[3,2-g][1]benzopyran-7-one, 2,3-dihydro-2-(1-hydroxy-1-methylethyl)-, (S)-(+)-
(+)-Marmesin
Marmesin
S-(+)-Marmesin
7H-Furo[3,2-g][1]benzopyran-7-one, 2,3-dihydro-2-(1-hydroxy-1-methylethyl)-, (+)-
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/h3-5,7,12,1

InchiKey: FWYSBEAFFPBAQU-GFCCVEGCSA-N

Formula: C14H14O4

SMILES: CC(C)(O)C1Cc2cc3ccc(=O)oc3cc2O1

Mol. weight [g/mol]: 246.26

CAS: 13849-08-6

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	2322.00		NIST Webbook
rinpol	2322.00		NIST Webbook

Sources

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=C13849086&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices