

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/h3-5,7,12,14
InchiKey:	FWYSBEAFFPBAQU-GFCCVEGCSA-N
Formula:	C14H14O4
SMILES:	<chem>CC(C)(O)C1Cc2cc3ccc(=O)oc3cc2O1</chem>
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

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