

2-Isopropenyl-2,3-dihydrofuro[3,2-g]chromen-7-one

Inchi: InChI=1S/C14H12O3/c1-8(2)11-6-10-5-9-3-4-14(15)17-12(9)7-13(10)16-11/h3-5,7,11H,1
InchiKey: VMWUHWZFDITAOL-UHFFFAOYSA-N
Formula: C14H12O3
SMILES: C=C(C)C1Cc2cc3ccc(=O)oc3cc2O1
Mol. weight [g/mol]: 228.24
CAS: 32375-25-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.05		Crippen Method
logp	2.673		Crippen Method
mcvol	167.350	ml/mol	McGowan Method
rinpol	2186.00		NIST Webbook
rinpol	2186.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=C32375250&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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