

2H-Furo[2,3-h]-1-benzopyran-2-one, 5-methoxy-

Other names:	Isobergapten Isobergaptene 5-Methoxyangelicin
Inchi:	InChI=1S/C12H8O4/c1-14-9-6-10-8(4-5-15-10)12-7(9)2-3-11(13)16-12/h2-6H,1H3
InchiKey:	AJSPSRWWZBBIOR-UHFFFAOYSA-N
Formula:	C12H8O4
SMILES:	<chem>COc1cc2occc2c2oc(=O)ccc12</chem>
Mol. weight [g/mol]:	216.19
CAS:	482-48-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.09		Crippen Method
logp	2.548		Crippen Method
mcvol	145.040	ml/mol	McGowan Method
rinpol	2016.00		NIST Webbook
rinpol	2016.00		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=C482484&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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