

2H-1-Benzopyran-2-one, 7-methoxy-6-(3-methyl-2-butenyl)-

Other names: Coumarin, 7-methoxy-6-(3-methyl-2-butenyl)-
Suberosin

Inchi: InChI=1S/C15H16O3/c1-10(2)4-5-11-8-12-6-7-15(16)18-14(12)9-13(11)17-3/h4,6-9H,5H

InchiKey: RSZDAYHEZSRVHS-UHFFFAOYSA-N

Formula: C15H16O3

SMILES: COc1cc2oc(=O)ccc2cc1CC=C(C)C

Mol. weight [g/mol]: 244.29

CAS: 581-31-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.46		Crippen Method
logp	3.310		Crippen Method
mcvol	192.300	ml/mol	McGowan Method

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=C581317&Units=SI>

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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