

2H-1-Benzopyran-2-one, 7-methoxy-8-(3-methylbutyl)-

Other names:

Dihydroosthol

8-Isopentyl-7-methoxy-2H-chromen-2-one

Coumarin, 8-(3-methylbutyl)-7-methoxy

Herniarin, 8-isoamyl-

Inchi: InChI=1S/C15H18O3/c1-10(2)4-7-12-13(17-3)8-5-11-6-9-14(16)18-15(11)12/h5-6,8-10H,

InchiKey: JUCKDULTLYEHAA-UHFFFAOYSA-N

Formula: C15H18O3

SMILES: COc1ccc2ccc(=O)oc2c1CCC(C)C

Mol. weight [g/mol]: 246.30

CAS: 6619-22-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.37		Crippen Method
logp	3.390		Crippen Method
mcvol	196.600	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C6619223&Units=SI>

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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