

5-isopentenylxy-7-methoxycoumarin

Inchi:	InChI=1S/C15H16O4/c1-10(2)6-7-18-13-8-11(17-3)9-14-12(13)4-5-15(16)19-14/h4-6,8-9
InchiKey:	HSJZJYCOXHKDBJ-UHFFFAOYSA-N
Formula:	C15H16O4
SMILES:	COc1cc(OCC=C(C)C)c2ccc(=O)oc2c1
Mol. weight [g/mol]:	260.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.20		Crippen Method
logp	3.147		Crippen Method
mcvol	198.170	ml/mol	McGowan Method
rinpol	2351.00		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=R422298&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

Latest version available from:

<https://www.chemeo.com/cid/84-982-9/5-isopentenylxy-7-methoxycoumarin.pdf>

Generated by Cheméo on 2025-12-22 13:11:17.622684493 +0000 UTC m=+6157275.152725146.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.