

2H-1-Benzopyran-2-one, 8-methoxy-

Other names:	Coumarin, 8-methoxy-
Inchi:	InChI=1S/C10H8O3/c1-12-8-4-2-3-7-5-6-9(11)13-10(7)8/h2-6H,1H3
InchiKey:	ODRDTKMYQDXVGG-UHFFFAOYSA-N
Formula:	C10H8O3
SMILES:	<chem>COc1cccc2ccc(=O)oc12</chem>
Mol. weight [g/mol]:	176.17
CAS:	2445-81-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.55		Crippen Method
logp	1.802		Crippen Method
mcvol	126.150	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2445810&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/53-051-6/2H-1-Benzopyran-2-one-8-methoxy.pdf>

Generated by Cheméo on 2025-12-05 14:37:32.99310397 +0000 UTC m=+4693650.523144625.

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