2H-1-Benzopyran-2-one, 7-methoxy-

Other names:	7-Methoxy-2H-1-benzopyran-2-one
	7-Methoxycoumarin
	7-Methyl ether derivative of Umbelliferone
	7-methoxychromen-2-one
	Ayapanin
	Coumarin, 7-methoxy-
	Herniarin
	Herniarine
	Methoxycourmarin, 7-
	Methylumbelliferone
	NSC 404559
	Umbelliferone, methyl ether
Inchi:	InChI=1S/C10H8O3/c1-12-8-4-2-7-3-5-10(11)13-9(7)6-8/h2-6H,1H3
InchiKey:	LIIALPBMIOVAHH-UHFFFAOYSA-N
Formula:	C10H8O3
SMILES:	COc1ccc2ccc(=O)oc2c1
Mol. weight [g/mol]:	176.17
CAS:	531-59-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.12		Aqueous Solubility Prediction Method
logp	1.802		Crippen Method
mcvol	126.150	ml/mol	McGowan Method
rinpol	1732.30		NIST Webbook
rinpol	1732.30		NIST Webbook
ripol	2910.00		NIST Webbook
ripol	2981.00		NIST Webbook
ripol	2910.00		NIST Webbook
ripol	2981.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C531599&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
ripol:	Polar retention indices