Scoparone

Other names:	2H-1-Benzopyran-2-one, 6,7-dimethoxy-
	Coumarin, 6,7-dimethoxy-
	Aesculetin dimethyl ether
	Escoparone
	Esculetin dimethyl ether
	Scoparon
	6,7-Dimethoxycoumarin
	6,7-Dimethylesculetin
	Dimethyl esculetin
	Benzopyran-2-one, 6,7-dimethoxy-
	Esculetin 6,7-dimethyl ether
	O,O-Dimethylesculetin
	O-Methylisoscopoletin
	O-Methylscopoletin
	Scopoletin methyl ether
	6,7-Dimethoxy-2H-chromen-2-one
	6,7-dimethoxy-2-benzopyrone
Inchi:	InChI=1S/C11H10O4/c1-13-9-5-7-3-4-11(12)15-8(7)6-10(9)14-2/h3-6H,1-2H3
InchiKey:	GUAFOGOEJLSQBT-UHFFFAOYSA-N
Formula:	C11H10O4
SMILES:	COc1cc2ccc(=O)oc2cc1OC
Mol. weight [g/mol]:	206.19
CAS:	120-08-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.67		Crippen Method
logp	1.810		Crippen Method
mcvol	146.110	ml/mol	McGowan Method
rinpol	2018.20		NIST Webbook
rinpol	2028.00		NIST Webbook
rinpol	1984.00		NIST Webbook
rinpol	2018.20		NIST Webbook
rinpol	1984.00		NIST Webbook

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=C120081&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