

4H-1-Benzopyran-4-one, 2-methyl-

Other names:	Chromone, 2-methyl- 2-Methyl-4-chromone 2-Methylchromone
Inchi:	InChI=1S/C10H8O2/c1-7-6-9(11)8-4-2-3-5-10(8)12-7/h2-6H,1H3
InchiKey:	PXPNSQMWWPLERM-UHFFFAOYSA-N
Formula:	C10H8O2
SMILES:	<chem>Cc1cc(=O)c2ccccc2o1</chem>
Mol. weight [g/mol]:	160.17
CAS:	5751-48-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.91		Crippen Method
logp	2.101		Crippen Method
mcvol	120.280	ml/mol	McGowan Method
rinpol	1318.00		NIST Webbook
rinpol	1318.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C5751484&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

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