2H-1-Benzopyran-2-one, 7,8-dihydroxy-6-methoxy-

Other names: Coumarin, 7,8-dihydroxy-6-methoxy
Fraxetin
7,8-dihydroxy-6-methoxy-2-benzopyrone
Inchi: InChI=1S/C10H8O5/c1-14-6-4-5-2-3-7(11)15-10(5)9(13)8(6)12/h2-4,12-13H,1H3
InchiKey: HAVWRBANWNTOJX-UHFFFAOYSA-N
Formula: C10H8O5
SMILES: COc1cc2ccc(=O)oc2c(O)c1O
Mol. weight [g/mol]: 208.17
CAS: 574-84-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.65		Crippen Method
logp	1.213		Crippen Method
mcvol	137.890	ml/mol	McGowan Method

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=C574845&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