Coumarin, 5-hydroxy-

Inchi: InChI=1S/C9H6O3/c10-7-2-1-3-8-6(7)4-5-9(11)12-8/h1-5,10H
InchiKey: CDHSCTCRBLLCBJ-UHFFFAOYSA-N
Formula: C9H6O3
SMILES: O=c1ccc2c(O)cccc2o1
Mol. weight [g/mol]: 162.14
CAS: 6093-67-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.98		Crippen Method
logp	1.499		Crippen Method
mcvol	112.060	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6093670&Units=SI
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

Legend

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