7-Hydroxycoumarin

Other names:	2H-1-Benzopyran-2-one, 7-hydroxy- 7 HC 7-Hydroxy-2-chromenone 7-Oxycoumarin 7-hydroxy-2H-chromen-2-one Coumarin, 7-hydroxy- Hydrangin Hydrangine NSC 19790 Skimmetin Skimmetine Umbelliferon umbelliferone
Inchi:	InChI=1S/C9H6O3/c10-7-3-1-6-2-4-9(11)12-8(6)5-7/h1-5,10H
InchiKey:	ORHBXUUXSCNDEV-UHFFFAOYSA-N
Formula:	C9H6O3
SMILES:	O=c1ccc2ccc(O)cc2o1
Mol. weight [g/mol]:	162.14
CAS:	93-35-6

Physical Properties

Property code	Value	Unit	Source
hfus	31.25	kJ/mol	Calorimetric and computational study of 7-hydroxycoumarin
log10ws	-5.98		Crippen Method
logp	1.499		Crippen Method
mcvol	112.060	ml/mol	McGowan Method
rinpol	1789.00		NIST Webbook
rinpol	1797.00		NIST Webbook
rinpol	1828.00		NIST Webbook
rinpol	1828.00		NIST Webbook
rinpol	1795.00		NIST Webbook
rinpol	1852.50		NIST Webbook
rinpol	1828.00		NIST Webbook
rinpol	1836.00		NIST Webbook

Sources

Equilibrium partitioning of drug molecules between aqueous and amino acid ester-based ionic liquids:	https://www.doi.org/10.1016/j.jct.2013.02.011
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C93356&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Calorimetric and computational study of 7-hydroxycoumarin:	https://www.doi.org/10.1016/j.jct.2011.04.015

Legend

hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices