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

Other names:	3-hydroxy-2H-1-benzopyran-2-one
	3-hydroxycoumarin
	4-Coumarinol
	4-Coumaryl alcohol
	4-Hydroxycoumarine
	4-hydroxy-2H-1-Benzopyran-2-one
	4-hydroxycoumarin
	Benzotetronic acid
	Coumarin, 4-hydroxy-
Inchi:	InChI=1S/C9H6O3/c10-7-5-9(11)12-8-4-2-1-3-6(7)8/h1-5,10H
InchiKey:	VXIXUWQIVKSKSA-UHFFFAOYSA-N
Formula:	C9H6O3
SMILES:	O=c1cc(O)c2ccccc2o1
Mol. weight [g/mol]:	162.14
CAS:	1076-38-6

Physical Properties

Property code	Value	Unit	Source
hfus	27.10	kJ/mol	Energetics of the isomers: 3- and 4-hydroxycoumarin
log10ws	-5.98		Crippen Method
logp	1.499		Crippen Method
mcvol	112.060	ml/mol	McGowan Method
rinpol	1652.00		NIST Webbook
rinpol	1656.00		NIST Webbook
rinpol	1665.00		NIST Webbook
tf	488.30	K	Solubilities of pharmaceutical and bioactive compounds in trihexyl(tetradecyl)phosphonium chloride ionic liquid

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Solubilities of pharmaceutical and bioactive compounds in trihexyl(tetradecyl)phosphonium chloride ionic liquid:	https://www.doi.org/10.1016/j.fluid.2015.03.053

Solubility studies on the system of trihexyl(tetradecyl)phosphonium bis[(trifluoromethyl)sulfonyl]amide) ionic liquid and pharmaceutical and bioactive compounds:	https://www.doi.org/10.1016/j.fluid.2014.10.033
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cripped Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of pharmaceutical compounds in ionic liquidsAna:	https://www.doi.org/10.1016/j.fluid.2013.07.020
Energetics of the isomers: 3- and 4-hydroxycoumarin:	https://www.doi.org/10.1016/j.jct.2010.06.003
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1076386&Units=SI

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
tf:	Normal melting (fusion) point