

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

<b>Other names:</b>	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-
<b>Inchi:</b>	InChI=1S/C9H6O3/c10-7-5-9(11)12-8-4-2-1-3-6(7)8/h1-5,10H
<b>InchiKey:</b>	VXIXUWQIVKSKSA-UHFFFAOYSA-N
<b>Formula:</b>	C9H6O3
<b>SMILES:</b>	O=c1cc(O)c2ccccc2o1
<b>Mol. weight [g/mol]:</b>	162.14
<b>CAS:</b>	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	1656.00		NIST Webbook
rinpol	1665.00		NIST Webbook
rinpol	1652.00		NIST Webbook
tf	488.30	K	Solubilities of pharmaceutical and bioactive compounds in trihexyl(tetradecyl)phosphonium chloride ionic liquid

## Sources

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>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C1076386&Units=SI>

**Energetics of the isomers: 3- and 4-hydroxycoumarin:** <https://www.doi.org/10.1016/j.jct.2010.06.003>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**Solubility of pharmaceutical compounds in ionic liquids:** <https://www.doi.org/10.1016/j.fluid.2013.07.020>  
**Solubilities of pharmaceutical and bioactive compounds in ionic liquids:** <https://www.doi.org/10.1016/j.fluid.2015.03.053>  
**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>

## 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  
**rinpola:** Non-polar retention indices  
**tf:** Normal melting (fusion) point

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