

3-Hydroxyflavone

Other names:	3-Hydroxy-2-phenylchromone 4H-1-Benzopyran-4-one, 3-hydroxy-2-phenyl- Flavon-3-ol Flavonol flavone, 3-hydroxy-
Inchi:	InChI=1S/C15H10O3/c16-13-11-8-4-5-9-12(11)18-15(14(13)17)10-6-2-1-3-7-10/h1-9,17H
InchiKey:	HVQAJTFOCKOKIN-UHFFFAOYSA-N
Formula:	C15H10O3
SMILES:	O=c1c(O)c(-c2ccccc2)oc2ccccc12
Mol. weight [g/mol]:	238.24
CAS:	577-85-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.58		Crippen Method
logp	3.166		Crippen Method
mcvol	172.840	ml/mol	McGowan Method
tf	443.60	K	Isothermal Thermogravimetric Study for Determining Sublimation Enthalpies of Some Hydroxyflavones

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Isothermal Thermogravimetric Study for Determining Sublimation Enthalpies of Some Hydroxyflavones:	https://www.doi.org/10.1021/acs.jced.7b01034
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C577855&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcpvol: McGowan's characteristic volume
tf: Normal melting (fusion) point

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