4H-1-Benzopyran-4-one, 3-hydroxy-2-phenyl-

Other names:	3-Hydroxy-2-phenylchromone
	3-hydroxyflavone
	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

Physical Properties

Property code	Value	Unit	Source
hf	-132.33	kJ/mol	Cheméo Relay (1.0)
ie	8.39	eV	Cheméo Relay (1.0)
log10ws	-3.52		Cheméo Relay (1.0)
logp	3.166		Crippen Method
mcvol	172.840	ml/mol	McGowan Method
pc	3820.10	kPa	Cheméo Relay (1.0, beta)
tb	646.97	K	Cheméo Relay (1.0)
tc	978.34	K	Cheméo Relay (1.0)
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/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Isothermal Thermogravimetric Study for Determining Sublimation Enthalpies of Some Hydroxyflavones:	https://www.doi.org/10.1021/acs.jced.7b01034
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C577855&Units=SI

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

hf:	Enthalpy of formation at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point