Hesperetin

Other names:	(S)-2,3-dihydro-5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)-4-benzopyrone
	2,3-Dihydro-5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)-4H-1-benzopyran-4-one
	2,3-Dihyro-5,7-dihyroxy-2-(3-hydroxy-4-methoxyphenyl)-4H-1-benzopyran-4-one
	(hesperitin)
	4H-1-Benzopyran-4-one, 2,3-dihydro-5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)-, (S)-
	Hesperitin
	Hesperitine
	NSC 57654
Inchi:	InChI=1S/C16H14O6/c1-21-13-3-2-8(4-10(13)18)14-7-12(20)16-11(19)5-9(17)6-15(16)22
InchiKey:	AIONOLUJZLIMTK-CQSZACIVSA-N
Formula:	C16H14O6
SMILES:	COc1ccc(C2CC(=O)c3c(O)cc(O)cc3O2)cc1O
Mol. weight [g/mol]:	302.28
CAS:	520-33-2

Physical Properties

Property code	Value	Unit	Source
gf	-439.52	kJ/mol	Joback Method
hf	-790.66	kJ/mol	Joback Method
hfus	46.56	kJ/mol	Joback Method
hvap	107.38	kJ/mol	Joback Method
log10ws	-5.35		Aqueous Solubility Prediction Method
logp	2.518		Crippen Method
mcvol	208.840	ml/mol	McGowan Method
pc	4379.97	kPa	Joback Method
rinpol	3014.60		NIST Webbook
rinpol	3014.60		NIST Webbook
tb	998.86	K	Joback Method
tc	1272.29	K	Joback Method
tf	501.48	K	Aqueous Solubility Prediction Method
vc	0.609	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	687.20	J/mol×K	998.86	Joback Method
cpg	702.76	J/mol×K	1044.43	Joback Method
cpg	718.87	J/mol×K	1090.00	Joback Method
cpg	735.80	J/mol×K	1135.58	Joback Method
cpg	753.81	J/mol×K	1181.15	Joback Method
cpg	773.17	J/mol×K	1226.72	Joback Method
cpg	794.16	J/mol×K	1272.29	Joback Method
hfust	35.90	kJ/mol	499.20	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C520332&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubility of Hesperetin in Mixed Solvents:	https://www.doi.org/10.1021/je400513s
Solubility of Hesperetin in Various Solvents from (288.2 to 323.2) K:	https://www.doi.org/10.1021/je800078j
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume