Quercetin

Other names:	2,(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-4H-1-benzopyran-4-one
	2-(3,4-Dihydroxyphenyl)-3,5,7-trihydroxy-4H-1-benzopyran-4-one
	2-(3,4-Dihydroxyphenyl)-3,5,7-trihydroxy-4H-1-benzopyran-4-one (quercetin)
	2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-4(4H)chromenone
	3,3',4',5,7-Pentahydroxyflavone
	3,5,7,3',4'-Pentahydroxyflavon
	3,5,7,3',4'-Pentahydroxyflavone
	4H-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-
	C.I. 75670
	C.I. Natural Yellow 10
	C.I. Natural red 1
	C.I. Natural yellow 10 & 13
	C.I. natural yellow 13
	Cyanidelonon 1522
	Cyanidenolon 1522
	Flavone, 3,3',4',5,7-pentahydroxy-
	Kvercetin
	Meletin
	NCI-C60106
	NSC 9219
	Quercetine
	Quercetol
	Quercitin
	Quertin
	Quertine
	Ritacetin
	Sophoretin
	T-Gelb bzw. grun 1
	Xanthaurine
Inchi:	InChI=1S/C15H10O7/c16-7-4-10(19)12-11(5-7)22-15(14(21)13(12)20)6-1-2-8(17)9(18)3-
InchiKey:	REFJWTPEDVJJIY-UHFFFAOYSA-N
Formula:	C15H10O7
SMILES:	O=c1c(O)c(-c2ccc(O)c(O)c2)oc2cc(O)cc(O)c12
Mol. weight [g/mol]:	302.24
CAS:	117-39-5

Physical Properties

Property code	Value	Unit	Source
hfus	41.50	kJ/mol	Solubility of Flavonoids in Organic Solvents
log10ws	-6.78		Crippen Method
logp	1.988		Crippen Method
mcvol	196.320	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	41.50	kJ/mol	595.20	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubilities of 7,8-Dihydroxyflavone and 3,3',4',5,7-Pentahydroxyflavone in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je030129z
Solubility of Flavonoids in Organic Solvents:	https://www.doi.org/10.1021/je7001094
Solubility of Quercetin in Water + Methanol and Water + Ethanol from (292.8 to 333.8) K:	https://www.doi.org/10.1021/je9010757
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C117395&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume