

QUERCERTIN

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
quercetin

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

Physical Properties

Property code	Value	Unit	Source
hfus	41.50	kJ/mol	Solubility of Flavonoids in Organic Solvents
log10ws	-3.35		Cheméo Relay (1.0)
logp	1.988		Crippen Method
mcvol	196.320	ml/mol	McGowan Method
tf	574.33	K	Cheméo Relay (1.0)

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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 Quercetin in Water + Methanol and Water + Ethanol from 292.15 to 333.15 K:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C117395&Units=SI
Cheméo Relay (1.0, beta):	https://www.doi.org/10.1021/je9010757
Solubility of Flavonoids in Organic Solvents:	https://www.doi.org/10.1021/je7001094

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
tf:	Normal melting (fusion) point

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