

Chrysin

Other names:

4H-1-benzopyran-4-one, 5,7-dihydroxy-2-phenyl-
5,7-Dihydroxy-2-phenyl-4H-1-benzoyran-4-one (chrysin)
5,7-dihydroxy-2-phenyl-4H-1-benzopyran-4-one
5,7-dihydroxy-2-phenyl-4H-benzo[b]pyran-4-one
5,7-dihydroxyflavone
Chryisine
flavone, 5,7-dihydroxy-

Inchi: InChI=1S/C15H10O4/c16-10-6-11(17)15-12(18)8-13(19-14(15)7-10)9-4-2-1-3-5-9/h1-8,1**InchiKey:** RTIXKCRFFJGDFG-UHFFFAOYSA-N**Formula:** C15H10O4**SMILES:** O=c1cc(-c2ccccc2)oc2cc(O)cc(O)c12**Mol. weight [g/mol]:** 254.24**CAS:** 480-40-0

Physical Properties

Property code	Value	Unit	Source
hfus	39.20	kJ/mol	Solubility of Flavonoids in Organic Solvents
log10ws	-8.13		Crippen Method
logp	2.871		Crippen Method
mcvol	178.710	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	39.20	kJ/mol	558.20	NIST Webbook

Sources

Solubility of Flavonoids in Organic Solvents:
McGowan Method:

<https://www.doi.org/10.1021/je7001094>

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C480400&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of chrysin in ethanol and water mixtures: <https://www.doi.org/10.1021/je5001654>

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

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