

4H-1-Benzopyran-4-one, 2,3-dihydro-5,7-dihydroxy-2-phenyl-, (S)-

Other names:

Dihydrochrysin

Galangin flavanone

Pinocembrin

4H-1-Benzopyran-4-one, 2,3-dihydro-5,7-dihydroxy-2-phenyl-, (-)-

5,7-Dihydroxyflavanone

Inchi: InChI=1S/C15H12O4/c16-10-6-11(17)15-12(18)8-13(19-14(15)7-10)9-4-2-1-3-5-9/h1-7,1

InchiKey: URFCJEUXXNAHFI-UHFFFAOYSA-N

Formula: C15H12O4

SMILES: O=C1CC(c2ccccc2)Oc2cc(O)cc(O)c21

Mol. weight [g/mol]: 256.25

CAS: 480-39-7

Physical Properties

Property code	Value	Unit	Source
gf	-178.69	kJ/mol	Joback Method
hf	-449.02	kJ/mol	Joback Method
hfus	37.39	kJ/mol	Joback Method
hvap	89.07	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	2.804		Crippen Method
mcpvol	183.010	ml/mol	McGowan Method
pc	4260.71	kPa	Joback Method
rinpol	2513.30		NIST Webbook
tb	867.96	K	Joback Method
tc	1147.06	K	Joback Method
tf	656.82	K	Joback Method
vc	0.569	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	560.27	J/mol×K	867.96	Joback Method
cpg	573.93	J/mol×K	914.48	Joback Method
cpg	587.16	J/mol×K	960.99	Joback Method

cpg	600.21	J/mol×K	1007.51	Joback Method
cpg	613.33	J/mol×K	1054.03	Joback Method
cpg	626.76	J/mol×K	1100.54	Joback Method
cpg	640.74	J/mol×K	1147.06	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C480397&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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

Latest version available from:

<https://www.chemeo.com/cid/91-330-4/4H-1-Benzopyran-4-one-2-3-dihydro-5-7-dihydroxy-2-phenyl-S.pdf>

Generated by Cheméo on 2024-04-19 21:39:56.528242715 +0000 UTC m=+15852045.448820028.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.