3-(4-hydroxyphenyl)-1-(2,4,6-trihydroxyphenyl)pro

Other names: phloretin
Inchi: InChI=1S/C15H14O5/c16-10-4-1-9(2-5-10)3-6-12(18)15-13(19)7-11(17)8-14(15)20/h1-2,
InchiKey: VGEREEWJJVICBM-UHFFFAOYSA-N
Formula: C15H14O5
SMILES: O=C(CCc1ccc(O)cc1)c1c(O)cc(O)cc1O
Mol. weight [g/mol]: 274.27

Physical Properties

Property code	Value	Unit	Source
gf	-447.16	kJ/mol	Joback Method
hf	-701.69	kJ/mol	Joback Method
hfus	56.44	kJ/mol	Solubilities of Three Flavonoids in Different Natural Deep Eutectic Solvents at T = (288.15 to 328.15) K
hvap	112.34	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	2.324		Crippen Method
mcvol	199.740	ml/mol	McGowan Method
pc	5594.19	kPa	Joback Method
tb	972.31	K	Joback Method
tc	1237.14	K	Joback Method
tf	808.46	K	Joback Method
tt	542.96	K	Solubilities of Three Flavonoids in Different Natural Deep Eutectic Solvents at T = (288.15 to 328.15) K
vc	0.529	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	625.03	J/mol×K	972.31	Joback Method
cpg	640.93	J/mol×K	1016.45	Joback Method
cpg	658.38	J/mol×K	1060.59	Joback Method

cpg	677.77	J/mol×K	1104.72	Joback Method
cpg	699.49	J/mol×K	1148.86	Joback Method
cpg	723.91	J/mol×K	1193.00	Joback Method
cpg	751.43	J/mol×K	1237.14	Joback Method
dvisc	3.8267684e-09	Pa×s	808.46	Joback Method
dvisc	2.3478871e-09	Pa×s	835.77	Joback Method
dvisc	1.4857567e-09	Pa×s	863.08	Joback Method
dvisc	9.6695962e-10	Pa×s	890.38	Joback Method
dvisc	6.4561098e-10	Pa×s	917.69	Joback Method
dvisc	4.4123803e-10	Pa×s	945.00	Joback Method
dvisc	3.0807758e-10	Pa×s	972.31	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubilities of Three Flavonoids in Different Natural Deep Eutectic Solvents at T = (288.15 to 328.15) K:	https://www.doi.org/10.1021/acs.jced.6b00552
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume