4H-1-Benzopyran-4-one, 2,3-dihydro-5-hydroxy-2-(4-hydroxyphenyl)-7-met (S)-

Other names: Flavanone, 4',5-dihydroxy-7-methoxy-, (S)-(-)-
Sakuranetin
4',5-dihydroxy-7-methoxyflavone

Inchi: InChI=1S/C16H14O5/c1-20-11-6-12(18)16-13(19)8-14(21-15(16)7-11)9-2-4-10(17)5-3-9/

InchiKey: DJOJDHGQRNZXQQ-UHFFFAOYSA-N

Formula: C16H14O5

SMILES: COc1cc(O)c2c(c1)OC(c1ccc(O)cc1)CC2=O

Mol. weight [g/mol]: 286.28

CAS: 2957-21-3

Physical Properties

Property code	Value	Unit	Source
gf	-284.90	kJ/mol	Joback Method
hf	-613.35	kJ/mol	Joback Method
hfus	40.78	kJ/mol	Joback Method
hvap	94.37	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	2.813		Crippen Method
mcvol	202.970	ml/mol	McGowan Method
pc	3628.97	kPa	Joback Method
rinpol	2877.30		NIST Webbook
rinpol	2877.30		NIST Webbook
tb	918.24	K	Joback Method
tc	1187.19	K	Joback Method
tf	702.84	K	Joback Method
vc	0.642	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	640.24	J/mol×K	918.24	Joback Method
cpg	654.09	J/mol×K	963.06	Joback Method
cpg	667.49	J/mol×K	1007.89	Joback Method
cpg	680.63	J/mol×K	1052.71	Joback Method

cpg	693.68	J/mol×K	1097.54	Joback Method
cpg	706.84	J/mol×K	1142.36	Joback Method
cpg	720.28	J/mol×K	1187.19	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C2957213&Units=SI

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