5-Hydroxy-4',7-dimethoxyflavanone

Other names: 7-Hydroxy-5-methoxy-2-(4-methoxyphenyl)chroman-4-one
Inchi: InChI=1S/C17H16O5/c1-20-11-5-3-10(4-6-11)15-9-14(19)17-13(18)7-12(21-2)8-16(17)22
InchiKey: CKEXCBVNKRHAMX-UHFFFAOYSA-N
Formula: C17H16O5
SMILES: COc1ccc(C2CC(=O)c3c(O)cc(OC)cc3O2)cc1
Mol. weight [g/mol]: 300.31
CAS: 69097-96-7

Physical Properties

Property code	Value	Unit	Source
gf	-236.49	kJ/mol	Joback Method
hf	-600.37	kJ/mol	Joback Method
hfus	38.38	kJ/mol	Joback Method
hvap	86.65	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.116		Crippen Method
mcvol	217.060	ml/mol	McGowan Method
pc	2665.27	kPa	Joback Method
rinpol	2700.10		NIST Webbook
rinpol	2700.10		NIST Webbook
tb	887.90	K	Joback Method
tc	1143.78	K	Joback Method
tf	637.14	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	675.44	J/mol×K	887.90	Joback Method
cpg	689.46	J/mol×K	930.55	Joback Method
cpg	702.30	J/mol×K	973.19	Joback Method
cpg	714.02	J/mol×K	1015.84	Joback Method
cpg	724.68	J/mol×K	1058.49	Joback Method
cpg	734.35	J/mol×K	1101.13	Joback Method

cpg	743.10	J/mol×K	1143.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C69097967&Units=SI
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

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