5,6,7,8,3',4'-Hexamethoxyflavanone

Inchi: InChI=1S/C21H24O8/c1-23-13-8-7-11(9-15(13)24-2)14-10-12(22)16-17(25-3)19(26-4)21
InchiKey: LTRBUBSPQISFFL-UHFFFAOYSA-N
Formula: C21H24O8
SMILES: COc1ccc(C2CC(=O)c3c(OC)c(OC)c(OC)c(OC)c3O2)cc1OC
Mol. weight [g/mol]: 404.41
CAS: 67549-69-3

Physical Properties

Property code	Value	Unit	Source
gf	-506.71	kJ/mol	Joback Method
hf	-1080.38	kJ/mol	Joback Method
hfus	46.16	kJ/mol	Joback Method
hvap	94.83	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	3.445		Crippen Method
mcvol	291.030	ml/mol	McGowan Method
pc	1481.57	kPa	Joback Method
rinpol	3034.80		NIST Webbook
rinpol	3034.80		NIST Webbook
tb	1008.40	K	Joback Method
tc	1245.17	K	Joback Method
tf	709.50	K	Joback Method
vc	1.081	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	957.99	J/mol×K	1008.40	Joback Method
cpg	967.93	J/mol×K	1047.86	Joback Method
cpg	975.37	J/mol×K	1087.32	Joback Method
cpg	980.24	J/mol×K	1126.78	Joback Method
cpg	982.44	J/mol×K	1166.25	Joback Method
cpg	981.85	J/mol×K	1205.71	Joback Method
cpg	978.39	J/mol×K	1245.17	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=C67549693&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