5-Hydroxy-3',4',6,7-tetramethoxyflavanone

Inchi: InChI=1S/C19H20O7/c1-22-12-6-5-10(7-14(12)23-2)13-8-11(20)17-15(26-13)9-16(24-3)1
InchiKey: SUPFYYVLYHYYGM-UHFFFAOYSA-N
Formula: C19H20O7
SMILES: COc1ccc(C2CC(=O)c3c(cc(OC)c(OC)c3O)O2)cc1OC
Mol. weight [g/mol]: 360.36
CAS: 98007-03-5

Physical Properties

Property code	Value	Unit	Source
gf	-448.91	kJ/mol	Joback Method
hf	-929.03	kJ/mol	Joback Method
hfus	45.16	kJ/mol	Joback Method
hvap	97.25	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.133		Crippen Method
mcvol	256.980	ml/mol	McGowan Method
pc	2079.33	kPa	Joback Method
rinpol	2983.50		NIST Webbook
tb	988.46	K	Joback Method
tc	1234.65	K	Joback Method
tf	729.18	K	Joback Method
vc	0.898	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	840.32	J/mol×K	988.46	Joback Method
cpg	852.45	J/mol×K	1029.49	Joback Method
cpg	863.05	J/mol×K	1070.52	Joback Method
cpg	872.11	J/mol×K	1111.55	Joback Method
cpg	879.64	J/mol×K	1152.59	Joback Method
cpg	885.64	J/mol×K	1193.62	Joback Method
cpg	890.11	J/mol×K	1234.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C98007035&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