3',4',5,6,7-Pentamethoxyflavanone

Inchi: InChI=1S/C20H22O7/c1-22-13-7-6-11(8-15(13)23-2)14-9-12(21)18-16(27-14)10-17(24-3
InchiKey: HFKPIRGXRKMHJS-UHFFFAOYSA-N
Formula: C20H22O7
SMILES: COc1ccc(C2CC(=O)c3c(cc(OC)c(OC)c3OC)O2)cc1OC
Mol. weight [g/mol]: 374.38
CAS: 66074-98-4

Physical Properties

Property code	Value	Unit	Source
gf	-400.50	kJ/mol	Joback Method
hf	-916.05	kJ/mol	Joback Method
hfus	42.77	kJ/mol	Joback Method
hvap	89.53	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	3.436		Crippen Method
mcvol	271.070	ml/mol	McGowan Method
pc	1639.10	kPa	Joback Method
rinpol	3059.20		NIST Webbook
rinpol	3059.20		NIST Webbook
tb	958.12	K	Joback Method
tc	1194.20	K	Joback Method
tf	663.48	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	875.66	J/mol×K	958.12	Joback Method
cpg	887.81	J/mol×K	997.47	Joback Method
cpg	897.86	J/mol×K	1036.81	Joback Method
cpg	905.73	J/mol×K	1076.16	Joback Method
cpg	911.37	J/mol×K	1115.51	Joback Method
cpg	914.69	J/mol×K	1154.85	Joback Method
cpg	915.62	J/mol×K	1194.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C66074984&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