Flavanone, 5-hydroxy-3',4',6,7,8-pentamethoxy-

Inchi: InChI=1S/C20H22O8/c1-23-12-7-6-10(8-14(12)24-2)13-9-11(21)15-16(22)18(25-3)20(27
InchiKey: XRMJVHGTNXEOHH-UHFFFAOYSA-N
Formula: C20H22O8
SMILES: COc1ccc(C2CC(=O)c3c(O)c(OC)c(OC)c(OC)c3O2)cc1OC
Mol. weight [g/mol]: 390.38
CAS: 15512-52-4

Physical Properties

Property code	Value	Unit	Source
gf	-555.12	kJ/mol	Joback Method
hf	-1093.36	kJ/mol	Joback Method
hfus	48.55	kJ/mol	Joback Method
hvap	102.54	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	3.142		Crippen Method
mcvol	276.940	ml/mol	McGowan Method
pc	1856.31	kPa	Joback Method
rinpol	3049.00		NIST Webbook
rinpol	3049.00		NIST Webbook
tb	1038.74	K	Joback Method
tc	1284.53	K	Joback Method
tf	775.20	K	Joback Method
vc	0.973	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	922.53	J/mol×K	1038.74	Joback Method
cpg	933.01	J/mol×K	1079.71	Joback Method
cpg	941.64	J/mol×K	1120.67	Joback Method
cpg	948.40	J/mol×K	1161.64	Joback Method
cpg	953.24	J/mol×K	1202.60	Joback Method
cpg	956.16	J/mol×K	1243.57	Joback Method
cpg	957.12	J/mol×K	1284.53	Joback Method

Sources

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=C15512524&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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