5,6,7,4'-Tetramethoxyflavanone

Inchi: InChI=1S/C19H20O6/c1-21-12-7-5-11(6-8-12)14-9-13(20)17-15(25-14)10-16(22-2)18(23
InchiKey: AENXIAWIJGWYCP-UHFFFAOYSA-N
Formula: C19H20O6
SMILES: COc1ccc(C2CC(=O)c3c(cc(OC)c(OC)c3OC)O2)cc1
Mol. weight [g/mol]: 344.36
CAS: 2569-77-9

Physical Properties

Property code	Value	Unit	Source
gf	-294.29	kJ/mol	Joback Method
hf	-751.72	kJ/mol	Joback Method
hfus	39.38	kJ/mol	Joback Method
hvap	84.23	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	3.427		Crippen Method
mcvol	251.110	ml/mol	McGowan Method
pc	1823.17	kPa	Joback Method
rinpol	2905.80		NIST Webbook
tb	907.84	K	Joback Method
tc	1146.22	K	Joback Method
tf	617.46	K	Joback Method
vc	0.932	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.27	J/mol×K	907.84	Joback Method
cpg	806.07	J/mol×K	947.57	Joback Method
cpg	818.04	J/mol×K	987.30	Joback Method
cpg	828.13	J/mol×K	1027.03	Joback Method
cpg	836.30	J/mol×K	1066.76	Joback Method
cpg	842.49	J/mol×K	1106.49	Joback Method
cpg	846.66	J/mol×K	1146.22	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2569779&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

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