2'-Hydroxy-3,3',4,4',5',6'-hexamethoxy-chalcone

Inchi: InChI=1S/C21H24O8/c1-24-14-10-8-12(11-15(14)25-2)7-9-13(22)16-17(23)19(27-4)21(2
InchiKey: YJWMUOUYEWHGFK-VQHVLOKHSA-N
Formula: C21H24O8
SMILES: COc1ccc(C=CC(=O)c2c(O)c(OC)c(OC)c(OC)c2OC)cc1OC
Mol. weight [g/mol]: 404.41
CAS: 78417-27-3

Physical Properties

Property code	Value	Unit	Source
gf	-540.34	kJ/mol	Joback Method
hf	-1038.52	kJ/mol	Joback Method
hfus	50.61	kJ/mol	Joback Method
hvap	105.04	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	3.340		Crippen Method
mcvol	297.590	ml/mol	McGowan Method
pc	1600.00	kPa	Joback Method
rinpol	3220.50		NIST Webbook
tb	1036.29	K	Joback Method
tc	1273.60	K	Joback Method
tf	744.34	K	Joback Method
vc	1.056	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	950.71	J/mol×K	1036.29	Joback Method
cpg	961.68	J/mol×K	1075.84	Joback Method
cpg	971.12	J/mol×K	1115.39	Joback Method
cpg	979.02	J/mol×K	1154.94	Joback Method
cpg	985.38	J/mol×K	1194.50	Joback Method
cpg	990.19	J/mol×K	1234.05	Joback Method
cpg	993.44	J/mol×K	1273.60	Joback Method
dvisc	0.0000039	Pa×s	744.34	Joback Method

dvisc	0.0000024	Pa×s	793.00	Joback Method
dvisc	0.0000016	Pa×s	841.66	Joback Method
dvisc	0.0000011	Pa×s	890.31	Joback Method
dvisc	0.0000008	Pa×s	938.97	Joback Method
dvisc	0.0000006	Pa×s	987.63	Joback Method
dvisc	0.0000005	Pa×s	1036.29	Joback Method

Sources

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=C78417273&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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

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