

2'-Hydroxy-4,4',5',6'-tetramethoxychalcone

Inchi:	InChI=1S/C19H20O6/c1-22-13-8-5-12(6-9-13)7-10-14(20)17-15(21)11-16(23-2)18(24-3)
InchiKey:	FRISOFZUHCOQEC-JXMROGBWSA-N
Formula:	C19H20O6
SMILES:	<chem>COc1ccc(C=CC(=O)c2c(O)cc(OC)c(OC)c2OC)cc1</chem>
Mol. weight [g/mol]:	344.36
CAS:	41929-26-4

Physical Properties

Property code	Value	Unit	Source
gf	-327.92	kJ/mol	Joback Method
hf	-709.86	kJ/mol	Joback Method
hfus	43.83	kJ/mol	Joback Method
hvap	94.45	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	3.323		Crippen Method
mcvol	257.670	ml/mol	McGowan Method
pc	1985.89	kPa	Joback Method
rinpol	2994.20		NIST Webbook
tb	935.73	K	Joback Method
tc	1169.80	K	Joback Method
tf	652.30	K	Joback Method
vc	0.907	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	784.57	J/molxK	935.73	Joback Method
cpg	839.07	J/molxK	1130.79	Joback Method
cpg	830.04	J/molxK	1091.78	Joback Method
cpg	820.12	J/molxK	1052.76	Joback Method
cpg	809.26	J/molxK	1013.75	Joback Method
cpg	797.42	J/molxK	974.74	Joback Method
cpg	847.25	J/molxK	1169.80	Joback Method
dvisc	0.0000014	Paxs	935.73	Joback Method

dvisc	0.0000018	Paxs	888.49	Joback Method
dvisc	0.0000025	Paxs	841.25	Joback Method
dvisc	0.0000036	Paxs	794.02	Joback Method
dvisc	0.0000055	Paxs	746.78	Joback Method
dvisc	0.0000088	Paxs	699.54	Joback Method
dvisc	0.0000150	Paxs	652.30	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C41929264&Units=SI

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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