2-hydroxyl-tetramethoxy-acetophenone

Inchi: InChI=1S/C12H16O6/c1-6(13)7-8(14)10(16-3)12(18-5)11(17-4)9(7)15-2/h14H,1-5H3
InchiKey: HLANCZONPAGXFJ-UHFFFAOYSA-N
Formula: C12H16O6
SMILES: COc1c(O)c(C(C)=O)c(OC)c(OC)c1OC
Mol. weight [g/mol]: 256.25

Physical Properties

Property code	Value	Unit	Source
gf	-579.49	kJ/mol	Joback Method
hf	-919.13	kJ/mol	Joback Method
hfus	31.46	kJ/mol	Joback Method
hvap	76.63	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	1.629		Crippen Method
mcvol	187.100	ml/mol	McGowan Method
pc	2616.41	kPa	Joback Method
rinpol	1732.00		NIST Webbook
tb	744.73	K	Joback Method
tc	957.24	K	Joback Method
tf	552.07	K	Joback Method
vc	0.643	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	519.08	J/mol×K	744.73	Joback Method
cpg	531.54	J/mol×K	780.15	Joback Method
cpg	543.32	J/mol×K	815.57	Joback Method
cpg	554.40	J/mol×K	850.98	Joback Method
cpg	564.78	J/mol×K	886.40	Joback Method
cpg	574.44	J/mol×K	921.82	Joback Method
cpg	583.37	J/mol×K	957.24	Joback Method
dvisc	0.0000551	Pa×s	552.07	Joback Method
dvisc	0.0000351	Pa×s	584.18	Joback Method

dvisc	0.0000235	Pa×s	616.29	Joback Method
dvisc	0.0000163	Pa×s	648.40	Joback Method
dvisc	0.0000118	Pa×s	680.51	Joback Method
dvisc	0.0000087	Pa×s	712.62	Joback Method
dvisc	0.0000066	Pa×s	744.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R301547&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
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