2,3,4,6-tetramethoxy-acetophenone

Inchi: InChI=1S/C12H16O5/c1-7(13)10-8(14-2)6-9(15-3)11(16-4)12(10)17-5/h6H,1-5H3
InchiKey: FENZKGOUICFKMZ-UHFFFAOYSA-N
Formula: C12H16O5
SMILES: COc1cc(OC)c(C(C)=O)c(OC)c1OC
Mol. weight [g/mol]: 240.25

Physical Properties

Property code	Value	Unit	Source
gf	-424.87	kJ/mol	Joback Method
hf	-741.82	kJ/mol	Joback Method
hfus	25.67	kJ/mol	Joback Method
hvap	63.62	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	1.924		Crippen Method
mcvol	181.230	ml/mol	McGowan Method
pc	2258.96	kPa	Joback Method
rinpol	1670.00		NIST Webbook
tb	664.11	K	Joback Method
tc	867.85	K	Joback Method
tf	440.35	K	Joback Method
vc	0.677	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	468.52	J/mol×K	664.11	Joback Method
cpg	482.27	J/mol×K	698.07	Joback Method
cpg	495.35	J/mol×K	732.02	Joback Method
cpg	507.73	J/mol×K	765.98	Joback Method
cpg	519.37	J/mol×K	799.94	Joback Method
cpg	530.23	J/mol×K	833.90	Joback Method
cpg	540.27	J/mol×K	867.85	Joback Method
dvisc	0.0004089	Pa×s	440.35	Joback Method
dvisc	0.0002867	Pa×s	477.64	Joback Method

dvisc	0.0002116	Pa×s	514.94	Joback Method
dvisc	0.0001627	Pa×s	552.23	Joback Method
dvisc	0.0001293	Pa×s	589.52	Joback Method
dvisc	0.0001057	Pa×s	626.82	Joback Method
dvisc	0.0000883	Pa×s	664.11	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R301512&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