2',3',4' Trimethoxyacetophenone

Other names:	2,3,4-Trimethoxyacetophenone
	Ethanone, 1-(2,3,4-trimethoxyphenyl)-
	1-(2,3,4-trimethoxyphenyl)-ethanone
Inchi:	InChI=1S/C11H14O4/c1-7(12)8-5-6-9(13-2)11(15-4)10(8)14-3/h5-6H,1-4H3
InchiKey:	PKNAATJMQOUREZ-UHFFFAOYSA-N
Formula:	C11H14O4
SMILES:	COc1ccc(C(C)=O)c(OC)c1OC
Mol. weight [g/mol]:	210.23
CAS:	13909-73-4

Physical Properties

Property code	Value	Unit	Source
gf	-318.66	kJ/mol	Joback Method
hf	-577.49	kJ/mol	Joback Method
hfus	22.28	kJ/mol	Joback Method
hvap	58.32	kJ/mol	Joback Method
log10ws	-2.49		Crippen Method
logp	1.915		Crippen Method
mcvol	161.270	ml/mol	McGowan Method
pc	2561.10	kPa	Joback Method
ripol	2239.00		NIST Webbook
ripol	2239.00		NIST Webbook
tb	569.20	K	NIST Webbook
tc	821.66	K	Joback Method
tf	394.33	K	Joback Method
vc	0.604	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.23	J/mol×K	613.83	Joback Method
cpg	407.53	J/mol×K	648.47	Joback Method
cpg	420.23	J/mol×K	683.11	Joback Method
cpg	432.28	J/mol×K	717.75	Joback Method

cpg	443.68	J/mol×K	752.39	Joback Method
cpg	454.40	J/mol×K	787.02	Joback Method
cpg	464.40	J/mol×K	821.66	Joback Method
dvisc	0.0006543	Pa×s	394.33	Joback Method
dvisc	0.0004404	Pa×s	430.91	Joback Method
dvisc	0.0003154	Pa×s	467.50	Joback Method
dvisc	0.0002371	Pa×s	504.08	Joback Method
dvisc	0.0001853	Pa×s	540.66	Joback Method
dvisc	0.0001494	Pa×s	577.25	Joback Method
dvisc	0.0001235	Pa×s	613.83	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=C13909734&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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