Ethanone, 1-(2,4,6-trimethylphenyl)-

Other names:	Acetophenone, 2',4',6'-trimethyl-
	Acetomesitylene
	Mesityl methyl ketone
	Methyl 2,4,6-trimethylphenyl ketone
	2',4',6'-Trimethylacetophenone
	1-(2,4,6-Trimethylphenyl)-ethanone
	2,4,6-Trimethyl-acetophenone
	Acetylmesitylene
	1,3,5-Trimethyl-2-acetylbenzene
	1-(2,4,6-Trimethylphenyl)-1-ethanone
	1-Acetyl-2,4,6-trimethylbenzene
	Methyl mesityl ketone
	NSC 65636
Inchi:	InChI=1S/C11H14O/c1-7-5-8(2)11(10(4)12)9(3)6-7/h5-6H,1-4H3
InchiKey:	XWCIICLTKWRWCI-UHFFFAOYSA-N
Formula:	C11H14O
SMILES:	CC(=O)c1c(C)cc(C)cc1C
Mol. weight [g/mol]:	162.23
CAS:	1667-01-2

Physical Properties

Property code	Value	Unit	Source
chl	-6062.20 ± 2.90	kJ/mol	NIST Webbook
ea	0.49 ± 0.04	eV	NIST Webbook
gf	-3.66	kJ/mol	Joback Method
hf	-205.00 ± 4.20	kJ/mol	NIST Webbook
hfl	-267.00 ± 3.00	kJ/mol	NIST Webbook
hfus	18.72	kJ/mol	Joback Method
hvap	62.00	kJ/mol	NIST Webbook
hvap	62.30 ± 2.10	kJ/mol	NIST Webbook
ie	8.50	eV	NIST Webbook
ie	8.20	eV	NIST Webbook
log10ws	-3.56		Crippen Method
logp	2.814		Crippen Method
mcvol	143.660	ml/mol	McGowan Method
pc	2698.60	kPa	Joback Method
tb	508.70	K	NIST Webbook

tc	761.35	K	Joback Method
tf	327.64	K	Joback Method
vc	0.549	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.26	J/mol×K	546.57	Joback Method
cpg	335.10	J/mol×K	582.37	Joback Method
cpg	348.22	J/mol×K	618.16	Joback Method
cpg	360.64	J/mol×K	653.96	Joback Method
cpg	372.39	J/mol×K	689.76	Joback Method
cpg	383.47	J/mol×K	725.55	Joback Method
cpg	393.90	J/mol×K	761.35	Joback Method
dvisc	0.0013575	Pa×s	327.64	Joback Method
dvisc	0.0008654	Pa×s	364.13	Joback Method
dvisc	0.0005988	Pa×s	400.62	Joback Method
dvisc	0.0004406	Pa×s	437.10	Joback Method
dvisc	0.0003399	Pa×s	473.59	Joback Method
dvisc	0.0002722	Pa×s	510.08	Joback Method
dvisc	0.0002245	Pa×s	546.57	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	513.20	K	98.00	NIST Webbook

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=C1667012&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume