Ethanone, 1-(2,4,5-trimethylphenyl)-

Other names:	Acetophenone, 2',4',5'-trimethyl-
	2',4',5'-Trimethylacetophenone
	1-(2,4,5-Trimethylphenyl)-ethanone
	2,4,5-Trimethyl-acetophenone
	1-(2,4,5-trimethylphenyl)ethan-1-one
Inchi:	InChI=1S/C11H14O/c1-7-5-9(3)11(10(4)12)6-8(7)2/h5-6H,1-4H3
InchiKey:	GENBEGZNCBFHSU-UHFFFAOYSA-N
Formula:	C11H14O
SMILES:	CC(=O)c1cc(C)c(C)cc1C
Mol. weight [g/mol]:	162.23
CAS:	2040-07-5

Physical Properties

Property code	Value	Unit	Source
chl	-6077.30 ± 4.20	kJ/mol	NIST Webbook
gf	-3.66	kJ/mol	Joback Method
hf	-189.00 ± 5.00	kJ/mol	NIST Webbook
hfl	-252.00 ± 4.60	kJ/mol	NIST Webbook
hfus	18.72	kJ/mol	Joback Method
hvap	63.00	kJ/mol	NIST Webbook
hvap	63.20 ± 2.10	kJ/mol	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	519.70	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	383.47	J/mol×K	725.55	Joback Method
cpg	372.39	J/mol×K	689.76	Joback Method
cpg	360.64	J/mol×K	653.96	Joback Method
cpg	348.22	J/mol×K	618.16	Joback Method
cpg	335.10	J/mol×K	582.37	Joback Method
cpg	393.90	J/mol×K	761.35	Joback Method
dvisc	0.0002245	Pa×s	546.57	Joback Method
dvisc	0.0002722	Pa×s	510.08	Joback Method
dvisc	0.0003399	Pa×s	473.59	Joback Method
dvisc	0.0004406	Pa×s	437.10	Joback Method
dvisc	0.0005988	Pa×s	400.62	Joback Method
dvisc	0.0008654	Pa×s	364.13	Joback Method
dvisc	0.0013575	Pa×s	327.64	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2040075&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

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
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
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume