Ethanone, 1-(2-methylphenyl)-

Other names:	1-(2-Methylphenyl)ethanone
	2'-Methylacetylphenone
	2'-methylacetophenone
	2-Acetyltoluene
	2-methylacetophenone
	Acetophenone, 2'-methyl-
	Methyl 2-methylphenyl ketone
	NSC 84233
	acetophenone, 2-methyl-
	methyl o-tolyl ketone
	o-Acetyltoluene
	o-Methylacetophenone
Inchi:	InChI=1S/C9H10O/c1-7-5-3-4-6-9(7)8(2)10/h3-6H,1-2H3
InchiKey:	YXWWHNCQZBVZPV-UHFFFAOYSA-N
Formula:	C9H10O
SMILES:	CC(=O)c1ccccc1C
Mol. weight [g/mol]:	134.18
CAS:	577-16-2

Physical Properties

Property code	Value	Unit	Source
gf	-1.24	kJ/mol	Joback Method
hf	-116.61	kJ/mol	Joback Method
hfus	14.32	kJ/mol	Joback Method
hvap	45.31	kJ/mol	Joback Method
ie	8.90	eV	NIST Webbook
ie	9.15	eV	NIST Webbook
ie	9.27 ± 0.01	eV	NIST Webbook
log10ws	-2.61		Crippen Method
logp	2.198		Crippen Method
mcvol	115.480	ml/mol	McGowan Method
pc	3448.03	kPa	Joback Method
rinpol	1108.00		NIST Webbook
rinpol	1112.00		NIST Webbook
rinpol	1139.00		NIST Webbook
rinpol	1112.00		NIST Webbook
rinpol	1112.40		NIST Webbook

rinpol	1181.20		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1128.60		NIST Webbook
rinpol	1133.70		NIST Webbook
rinpol	1181.20		NIST Webbook
rinpol	1177.70		NIST Webbook
rinpol	1174.60		NIST Webbook
rinpol	1124.70		NIST Webbook
rinpol	1113.10		NIST Webbook
rinpol	1124.00		NIST Webbook
rinpol	1112.40		NIST Webbook
ripol	1738.00		NIST Webbook
ripol	1686.00		NIST Webbook
ripol	1690.00		NIST Webbook
tb	487.20	K	NIST Webbook
tc	710.50	K	Joback Method
tf	280.06	K	Joback Method
vc	0.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.20	J/mol×K	710.50	Joback Method
cpg	233.60	J/mol×K	490.85	Joback Method
cpg	246.11	J/mol×K	527.46	Joback Method
cpg	257.89	J/mol×K	564.07	Joback Method
cpg	268.96	J/mol×K	600.67	Joback Method
cpg	279.35	J/mol×K	637.28	Joback Method
cpg	289.09	J/mol×K	673.89	Joback Method
dvisc	0.0002611	Pa×s	490.85	Joback Method
dvisc	0.0021873	Pa×s	280.06	Joback Method
dvisc	0.0012598	Pa×s	315.19	Joback Method
dvisc	0.0008105	Pa×s	350.32	Joback Method
dvisc	0.0005651	Pa×s	385.45	Joback Method
dvisc	0.0004185	Pa×s	420.59	Joback Method
dvisc	0.0003246	Pa×s	455.72	Joback Method
hvapt	58.90	kJ/mol	298.15	Calorimetric study of 20-methylacetophenone and 40-methylacetophenone

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Calorimetric study of 20-methylacetophenone and 40-methylacetophenone:	https://www.doi.org/10.1016/j.jct.2012.08.034
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=C577162&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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