ETHANONE, 1-(3-METHYLPHENYL)-

Other names: 1-(3-Methylphenyl)-ethanone
3'-methylacetophenone
3-methylacetophenone
Acetophenone, 3'-methyl-
Acetophenone, m-methyl-
m-Methylacetophenone
methyl m-tolyl ketone

Inchi: InChI=1S/C9H10O/c1-7-4-3-5-9(6-7)8(2)10/h3-6H,1-2H3

InchiKey: FSPSELPMWGWDRY-UHFFFAOYSA-N

Formula: C9H10O

SMILES: CC(=O)c1cccc(C)c1

Mol. weight [g/mol]: 134.18

Physical Properties

Property code	Value	Unit	Source
af	0.4366		Cheméo Relay (1.0)
affp	868.20	kJ/mol	NIST Webbook
basg	836.40	kJ/mol	NIST Webbook
gf	-1.24	kJ/mol	Joback Method
hf	-135.18	kJ/mol	Cheméo Relay (1.0)
hfus	14.32	kJ/mol	Joback Method
hvap	62.21	kJ/mol	Cheméo Relay (1.0)
ie	9.14	eV	NIST Webbook
ie	9.15 ± 0.05	eV	NIST Webbook
ie	8.85	eV	NIST Webbook
ie	9.24 ± 0.02	eV	NIST Webbook
log10ws	-2.15		Cheméo Relay (1.0)
logp	2.198		Crippen Method
mcvol	115.480	ml/mol	McGowan Method
pc	3448.03	kPa	Joback Method
rinpol	1191.88		NIST Webbook
rinpol	1176.00		NIST Webbook
rinpol	1182.50		NIST Webbook
rinpol	1148.30		NIST Webbook
rinpol	1192.00		NIST Webbook
rinpol	1171.70		NIST Webbook
rinpol	1132.00		NIST Webbook

rinpol	1156.00		NIST Webbook
rinpol	1175.00		NIST Webbook
rinpol	1182.00		NIST Webbook
rinpol	1148.00		NIST Webbook
rinpol	1164.30		NIST Webbook
rinpol	1147.00		NIST Webbook
rinpol	1148.30		NIST Webbook
rinpol	1168.90		NIST Webbook
rinpol	1161.70		NIST Webbook
rinpol	1149.50		NIST Webbook
ripol	1786.00		NIST Webbook
ripol	1804.00		NIST Webbook
tb	493.20	K	NIST Webbook
tc	710.65	K	Cheméo Relay (1.0)
tf	270.45	K	Cheméo Relay (1.0)
vc	0.428	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	233.60	J/mol×K	490.85	Joback Method
cpg	298.20	J/mol×K	710.50	Joback Method
cpg	289.09	J/mol×K	673.89	Joback Method
cpg	279.35	J/mol×K	637.28	Joback Method
cpg	268.96	J/mol×K	600.67	Joback Method
cpg	257.89	J/mol×K	564.07	Joback Method
cpg	246.11	J/mol×K	527.46	Joback Method
dvisc	0.0005651	Pa×s	385.45	Joback Method
dvisc	0.0002611	Pa×s	490.85	Joback Method
dvisc	0.0003246	Pa×s	455.72	Joback Method
dvisc	0.0004185	Pa×s	420.59	Joback Method
dvisc	0.0021873	Pa×s	280.06	Joback Method
dvisc	0.0008105	Pa×s	350.32	Joback Method
dvisc	0.0012598	Pa×s	315.19	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source

tbrp	382.20	K	1.60	NIST Webbook

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Henry s Law Constants of Some Aromatic Aldehydes and Ketones Measured by an Internal Standard Method:	https://www.doi.org/10.1021/je700612b
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C585740&Units=SI

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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