3'-METHOXYACETOPHENONE

Other names: 1-(3-methoxyphenyl)ethanone
1-Acetyl-3-methoxybenzene
3-Acetylanisole
3-Methoxy-1-acetylbenzene
3-methoxyacetophenone
Acetophenone, 3'-methoxy-
Acetophenone, m-methoxy-
Ethanone, 1-(3-methoxyphenyl)-
Methyl 3-methoxyphenyl ketone
NSC 65593
m-Acetanisole
m-Acetylanisole
m-Metoxyacetophenone
m-methoxyacetophenone
meta-Methoxyacetophenone
methyl (3-methoxyphenyl) ketone

Inchi: InChI=1S/C9H10O2/c1-7(10)8-4-3-5-9(6-8)11-2/h3-6H,1-2H3

InchiKey: BAYUSCHCCGXLAY-UHFFFAOYSA-N

Formula: C9H10O2

SMILES: COc1cccc(C(C)=O)c1

Mol. weight [g/mol]: 150.18

Physical Properties

Property code	Value	Unit	Source
af	0.5016		Cheméo Relay (1.0)
affp	871.20	kJ/mol	NIST Webbook
basg	839.30	kJ/mol	NIST Webbook
gf	-106.24	kJ/mol	Joback Method
hf	-248.82	kJ/mol	Cheméo Relay (1.0)
hfus	15.50	kJ/mol	Joback Method
hvap	70.64	kJ/mol	Cheméo Relay (1.0)
ie	8.53 ± 0.05	eV	NIST Webbook
log10ws	-2.08		Cheméo Relay (1.0)
logp	1.898		Crippen Method
mcvol	121.350	ml/mol	McGowan Method
pc	3380.21	kPa	Joback Method
rinpol	1282.00		NIST Webbook

rinpol	1277.00		NIST Webbook
rinpol	1295.00		NIST Webbook
rinpol	1279.00		NIST Webbook
rinpol	1321.00		NIST Webbook
rinpol	1279.00		NIST Webbook
rinpol	1298.00		NIST Webbook
rinpol	1295.00		NIST Webbook
rinpol	1321.00		NIST Webbook
rinpol	1301.00		NIST Webbook
ripol	2148.00		NIST Webbook
ripol	2148.00		NIST Webbook
tb	513.20	K	NIST Webbook
tc	724.30	K	Cheméo Relay (1.0)
tf	295.59	K	Cheméo Relay (1.0)
vc	0.446	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.24	J/mol×K	513.27	Joback Method
cpg	320.16	J/mol×K	730.64	Joback Method
cpg	311.06	J/mol×K	694.41	Joback Method
cpg	301.35	J/mol×K	658.18	Joback Method
cpg	291.03	J/mol×K	621.95	Joback Method
cpg	280.07	J/mol×K	585.73	Joback Method
cpg	268.48	J/mol×K	549.50	Joback Method
dvisc	0.0004764	Pa×s	407.78	Joback Method
dvisc	0.0002227	Pa×s	513.27	Joback Method
dvisc	0.0002765	Pa×s	478.11	Joback Method
dvisc	0.0003552	Pa×s	442.94	Joback Method
dvisc	0.0017319	Pa×s	302.29	Joback Method
dvisc	0.0006754	Pa×s	372.62	Joback Method
dvisc	0.0010297	Pa×s	337.45	Joback Method
hvapt	67.80	kJ/mol	298.15	Standard molar enthalpy of formation of methoxyacetophenone isomers

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	398.70	K	1.60	NIST Webbook

Sources

Cheméo Relay (1.0):

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C586378&Units=SI

Standard molar enthalpy of formation of methoxyacetophenone isomers: https://www.doi.org/10.1016/j.jct.2014.03.027

Partition Coefficients of Organic Solutes between Supercritical Carbon Dioxide and Water: Experimental Measurements and Empirical Correlations: https://www.doi.org/10.1021/je030197l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume