2-Methoxy-1-phenyl-ethanone

Other names: 2-Methoxyacetophenone
«alpha»-methoxyacetophenone
Inchi: InChI=1S/C9H10O2/c1-11-7-9(10)8-5-3-2-4-6-8/h2-6H,7H2,1H3
InchiKey: YRNDGUSDBCARGC-UHFFFAOYSA-N
Formula: C9H10O2
SMILES: COCC(=O)c1ccccc1
Mol. weight [g/mol]: 150.17
CAS: 4079-52-1

Physical Properties

Property code	Value	Unit	Source
gf	-96.61	kJ/mol	Joback Method
hf	-237.36	kJ/mol	Joback Method
hfus	15.89	kJ/mol	Joback Method
hvap	47.06	kJ/mol	Joback Method
ie	8.60 ± 0.05	eV	NIST Webbook
log10ws	-1.64		Crippen Method
logp	1.516		Crippen Method
mcvol	121.350	ml/mol	McGowan Method
pc	3439.94	kPa	Joback Method
tb	508.29	K	Joback Method
tc	724.46	K	Joback Method
tf	289.77	K	Joback Method
vc	0.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.39	J/mol×K	508.29	Joback Method
cpg	269.00	J/mol×K	544.32	Joback Method
cpg	280.90	J/mol×K	580.35	Joback Method
cpg	292.11	J/mol×K	616.37	Joback Method
cpg	302.63	J/mol×K	652.40	Joback Method
cpg	312.50	J/mol×K	688.43	Joback Method

cpg	321.72	J/mol×K	724.46	Joback Method
dvisc	0.0023343	Pa×s	289.77	Joback Method
dvisc	0.0012799	Pa×s	326.19	Joback Method
dvisc	0.0007918	Pa×s	362.61	Joback Method
dvisc	0.0005347	Pa×s	399.03	Joback Method
dvisc	0.0003856	Pa×s	435.45	Joback Method
dvisc	0.0002925	Pa×s	471.87	Joback Method
dvisc	0.0002308	Pa×s	508.29	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	395.70	K	2.40	NIST Webbook

Sources

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=C4079521&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
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