

2-Methoxycyclohexanone

Other names:	Cyclohexanone, 2-methoxy-
Inchi:	InChI=1S/C7H12O2/c1-9-7-5-3-2-4-6(7)8/h7H,2-5H2,1H3
InchiKey:	JYJURPHZXCLFDX-UHFFFAOYSA-N
Formula:	C7H12O2
SMILES:	COC1CCCCC1=O
Mol. weight [g/mol]:	128.17
CAS:	7429-44-9

Physical Properties

Property code	Value	Unit	Source
gf	-195.08	kJ/mol	Joback Method
hf	-403.41	kJ/mol	Joback Method
hfus	6.42	kJ/mol	Joback Method
hvap	38.26	kJ/mol	Joback Method
ie	9.06	eV	NIST Webbook
log10ws	-1.13		Crippen Method
logp	1.144		Crippen Method
mcvol	106.070	ml/mol	McGowan Method
pc	3598.56	kPa	Joback Method
tb	469.35	K	Joback Method
tc	691.07	K	Joback Method
tf	266.48	K	Joback Method
vc	0.386	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.23	J/molxK	469.35	Joback Method
cpg	243.63	J/molxK	506.30	Joback Method
cpg	258.46	J/molxK	543.26	Joback Method
cpg	272.67	J/molxK	580.21	Joback Method
cpg	286.25	J/molxK	617.16	Joback Method
cpg	299.17	J/molxK	654.12	Joback Method
cpg	311.39	J/molxK	691.07	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	458.20	K	100.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
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=C7429449&Units=SI

Legend

cpg:	Ideal gas heat capacity
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

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