Methoxyacetonitrile

Other names:	NCCH2OCH3
	Acetonitrile, methoxy-
Inchi:	InChI=1S/C3H5NO/c1-5-3-2-4/h3H2,1H3
InchiKey:	QKPVEISEHYYHRH-UHFFFAOYSA-N
Formula:	C3H5NO
SMILES:	COCC#N
Mol. weight [g/mol]:	71.08
CAS:	1738-36-9

Physical Properties

Property code	Value	Unit	Source
affp	758.10	kJ/mol	NIST Webbook
basg	727.40	kJ/mol	NIST Webbook
chl	-1217.70 ± 0.17	kJ/mol	NIST Webbook
gf	2.56	kJ/mol	Joback Method
hf	-35.65 ± 0.66	kJ/mol	NIST Webbook
hfl	-77.36 ± 0.21	kJ/mol	NIST Webbook
hfus	6.22	kJ/mol	Joback Method
hvap	41.70 ± 0.60	kJ/mol	NIST Webbook
hvap	41.71 ± 0.63	kJ/mol	NIST Webbook
ie	10.75	eV	NIST Webbook
log10ws	-0.03		Crippen Method
logp	0.156		Crippen Method
mcvol	60.380	ml/mol	McGowan Method
pc	4173.09	kPa	Joback Method
tb	392.54	K	Joback Method
tc	585.85	K	Joback Method
tf	210.79	K	Joback Method
vc	0.247	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	103.82	J/mol×K	392.54	Joback Method

cpg	108.46	J/mol×K	424.76	Joback Method
cpg	113.02	J/mol×K	456.98	Joback Method
cpg	117.47	J/mol×K	489.19	Joback Method
cpg	121.82	J/mol×K	521.41	Joback Method
cpg	126.06	J/mol×K	553.63	Joback Method
cpg	130.18	J/mol×K	585.85	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	391.30	K	97.50	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=C1738369&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp: Proton affinity
basg: Gas basicity
chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase 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