

Methyl isocyanide

Other names:	Methane, isocyano- Isocyanomethane Methyl isonitrile CH ₃ NC
Inchi:	InChI=1S/C2H3N/c1-3-2/h1H3
InchiKey:	ZRKSVHFXTRFQFL-UHFFFAOYSA-N
Formula:	C ₂ H ₃ N
SMILES:	[C-]#[N+]C
Mol. weight [g/mol]:	41.05
CAS:	593-75-9

Physical Properties

Property code	Value	Unit	Source
affp	839.10	kJ/mol	NIST Webbook
basg	806.60	kJ/mol	NIST Webbook
basg	848.60 ± 5.30	kJ/mol	NIST Webbook
chl	-1333.00	kJ/mol	NIST Webbook
chl	-1333.00	kJ/mol	NIST Webbook
gf	99.14	kJ/mol	Joback Method
hf	142.80	kJ/mol	NIST Webbook
hf	163.50 ± 7.20	kJ/mol	NIST Webbook
hfl	112.00	kJ/mol	NIST Webbook
hfl	132.70 ± 7.30	kJ/mol	NIST Webbook
hfus	2.44	kJ/mol	Joback Method
hvap	30.80	kJ/mol	NIST Webbook
hvap	30.80 ± 1.00	kJ/mol	NIST Webbook
ie	11.53 ± 0.04	eV	NIST Webbook
ie	11.24	eV	NIST Webbook
ie	11.24	eV	NIST Webbook
ie	11.27	eV	NIST Webbook
ie	11.32	eV	NIST Webbook
ie	11.50 ± 0.25	eV	NIST Webbook
ie	11.83	eV	NIST Webbook
log10ws	-2.43		Crippen Method
logp	0.535		Crippen Method
mvol	40.420	ml/mol	McGowan Method
pc	4856.20	kPa	Joback Method

ripol	1010.00		NIST Webbook
ripol	1010.00		NIST Webbook
ripol	1002.00		NIST Webbook
tb	347.24	K	Joback Method
tc	541.37	K	Joback Method
tf	228.15 ± 3.00	K	NIST Webbook
vc	0.173	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	56.48	J/mol×K	347.24	Joback Method
cpg	59.46	J/mol×K	379.59	Joback Method
cpg	62.33	J/mol×K	411.95	Joback Method
cpg	65.11	J/mol×K	444.30	Joback Method
cpg	67.79	J/mol×K	476.66	Joback Method
cpg	70.38	J/mol×K	509.01	Joback Method
cpg	72.87	J/mol×K	541.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C593759&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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