Methanimine

Inchi: InChI=1S/CH3N/c1-2/h2H,1H2
InchiKey: WDWDWGRYHDPSDS-UHFFFAOYSA-N
Formula: CH3N
SMILES: C=N
Mol. weight [g/mol]: 29.04
CAS: 2053-29-4

Physical Properties

Property code	Value	Unit	Source
affp	852.90	kJ/mol	NIST Webbook
basg	818.70	kJ/mol	NIST Webbook
gf	177.31	kJ/mol	Joback Method
hf	110.00 ± 8.00	kJ/mol	NIST Webbook
hf	110.00 ± 13.00	kJ/mol	NIST Webbook
hf	69.00 ± 8.00	kJ/mol	NIST Webbook
hvap	29.19	kJ/mol	Joback Method
ie	9.88 ± 0.07	eV	NIST Webbook
ie	10.00	eV	NIST Webbook
ie	10.70	eV	NIST Webbook
ie	9.97	eV	NIST Webbook
log10ws	-1.16		Crippen Method
logp	0.266		Crippen Method
mcvol	30.630	ml/mol	McGowan Method
tb	299.26	K	Joback Method
tf	187.09	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	33.80	J/mol×K	299.26	Joback Method
cpg	7.26	J/mol×K	100.12	Joback Method
cpg	7.26	J/mol×K	100.12	Joback Method
cpg	7.26	J/mol×K	100.12	Joback Method
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cpg	7.26	J/mol×K	100.12	Joback Method
cpg	7.26	J/mol×K	100.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2053294&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation 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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point