

CH3NHCH2CN

Other names:	Methylaminoacetonitrile Acetonitrile, (methylamino)- Glycinonitrile, N-methyl- N-Methylaminoacetonitrile Sarcosinonitrile
Inchi:	InChI=1S/C3H6N2/c1-5-3-2-4/h5H,3H2,1H3
InchiKey:	PVVRUUMHFWFQV-UHFFFAOYSA-N
Formula:	C3H6N2
SMILES:	CNCC#N
Mol. weight [g/mol]:	70.09
CAS:	5616-32-0

Physical Properties

Property code	Value	Unit	Source
affp	863.80	kJ/mol	NIST Webbook
basg	830.70	kJ/mol	NIST Webbook
gf	196.95	kJ/mol	Joback Method
hf	113.10	kJ/mol	Joback Method
hfus	10.13	kJ/mol	Joback Method
hvap	39.19	kJ/mol	Joback Method
log10ws	-0.13		Crippen Method
logp	-0.271		Crippen Method
mcvol	64.490	ml/mol	McGowan Method
pc	4339.67	kPa	Joback Method
tb	420.29	K	Joback Method
tc	618.43	K	Joback Method
tf	241.22	K	Joback Method
vc	0.265	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	116.36	J/mol×K	420.29	Joback Method
cpg	122.27	J/mol×K	453.31	Joback Method

cpg	127.93	J/mol×K	486.34	Joback Method
cpg	133.34	J/mol×K	519.36	Joback Method
cpg	138.50	J/mol×K	552.38	Joback Method
cpg	143.42	J/mol×K	585.41	Joback Method
cpg	148.11	J/mol×K	618.43	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5616320&Units=SI

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
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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