Propanenitrile, 3-(methylamino)-

Other names:	N-Methyl-«beta»-alaninenitrile 3-(Methylamino)propionitrile «beta»-Methylaminopropionitrile (2-Cyanoethyl)methyl amine N-«beta»-Cyanoethylmethylamine N-Methyl-«beta»-aminopropionitrile Propionitrile, 3-(methylamino)- 3-(N-Methylamino)propionitrile N-(2-Cyanoethyl)methylamine NSC 8399
Inchi:	InChI=1S/C4H8N2/c1-6-4-2-3-5/h6H,2,4H2,1H3
InchiKey:	UNIJBMUBHBAUET-UHFFFAOYSA-N
Formula:	C4H8N2
SMILES:	CNCCC#N
Mol. weight [g/mol]:	84.12
CAS:	693-05-0

Physical Properties

Property code	Value	Unit	Source
chl	-2776.60 ± 1.60	kJ/mol	NIST Webbook
gf	205.37	kJ/mol	Joback Method
hf	92.46	kJ/mol	Joback Method
hfl	59.20 ± 1.60	kJ/mol	NIST Webbook
hfus	12.72	kJ/mol	Joback Method
hvap	41.41	kJ/mol	Joback Method
log10ws	-0.55		Crippen Method
logp	0.119		Crippen Method
mcvol	78.580	ml/mol	McGowan Method
pc	3838.78	kPa	Joback Method
tb	443.17	K	Joback Method
tc	639.26	K	Joback Method
tf	252.49	K	Joback Method
vc	0.321	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	152.03	J/mol×K	443.17	Joback Method
cpg	159.42	J/mol×K	475.85	Joback Method
cpg	166.49	J/mol×K	508.53	Joback Method
cpg	173.24	J/mol×K	541.22	Joback Method
cpg	179.68	J/mol×K	573.90	Joback Method
cpg	185.81	J/mol×K	606.58	Joback Method
cpg	191.65	J/mol×K	639.26	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C693050&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

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
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
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume