3-Aminopropionitrile

Other names:	3-Aminopropanenitrile
	H2NCH2CH2CN
	«beta»-Aminoethyl cyanide
	«beta»-Aminopropionitrile
	Propanenitrile, 3-amino-
	«beta»-Alaninenitrile
	«beta»-Cyanoethylamine
	Aminopropionitrile
	BAPN
	Propionitrile, 3-amino-
	2-Cyanoethylamine
	NSC 40641
	3-aminopropiononitrile
Inchi:	InChI=1S/C3H6N2/c4-2-1-3-5/h1-2,4H2
InchiKey:	AGSPXMVUFBBBMO-UHFFFAOYSA-N
Formula:	C3H6N2
SMILES:	N#CCCN
Mol. weight [g/mol]:	70.09
CAS:	151-18-8

Physical Properties

Property code	Value	Unit	Source
affp	866.40	kJ/mol	NIST Webbook
basg	832.50	kJ/mol	NIST Webbook
gf	174.01	kJ/mol	Joback Method
hf	89.75	kJ/mol	NIST Webbook
hfus	10.23	kJ/mol	Joback Method
hvap	43.39	kJ/mol	Joback Method
log10ws	-0.38		Crippen Method
logp	-0.141		Crippen Method
mcvol	64.490	ml/mol	McGowan Method
pc	4602.62	kPa	Joback Method
rinpol	789.00		NIST Webbook
rinpol	789.00		NIST Webbook
tb	442.65	K	Joback Method
tc	651.61	K	Joback Method
tf	271.82	K	Joback Method

vc	0.259	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	122.82	J/mol×K	442.65	Joback Method
cpg	128.54	J/mol×K	477.48	Joback Method
cpg	134.00	J/mol×K	512.30	Joback Method
cpg	139.20	J/mol×K	547.13	Joback Method
cpg	144.15	J/mol×K	581.96	Joback Method
cpg	148.85	J/mol×K	616.79	Joback Method
cpg	153.31	J/mol×K	651.61	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	353.00 ± 1.00	K	2.10	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C151188&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume