3-Aminocrotononitrile

Other names:	«beta»-Aminocrotononitrile
	3-Aminocrotonitrile
	«beta»-Aminocrotonitrile
	2-Butenenitrile, 3-amino-
Inchi:	InChI=1S/C4H6N2/c1-4(6)2-3-5/h2H,6H2,1H3/b4-2+
InchiKey:	DELJOESCKJGFML-DUXPYHPUSA-N
Formula:	C4H6N2
SMILES:	CC(N)=CC#N
Mol. weight [g/mol]:	82.10
CAS:	1118-61-2

Physical Properties

Property code	Value	Unit	Source
gf	254.10	kJ/mol	Joback Method
hf	180.21	kJ/mol	Joback Method
hfus	11.71	kJ/mol	Joback Method
hvap	45.66	kJ/mol	Joback Method
log10ws	-1.15		Crippen Method
logp	0.372		Crippen Method
mcvol	74.280	ml/mol	McGowan Method
pc	4368.40	kPa	Joback Method
tb	469.57	K	Joback Method
tc	690.56	K	Joback Method
tf	264.05	K	Joback Method
vc	0.295	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	141.79	J/mol×K	469.57	Joback Method
cpg	148.41	J/mol×K	506.40	Joback Method
cpg	154.61	J/mol×K	543.23	Joback Method
cpg	160.41	J/mol×K	580.07	Joback Method
cpg	165.85	J/mol×K	616.90	Joback Method

cpg	170.95	J/mol×K	653.73	Joback Method
cpg	175.73	J/mol×K	690.56	Joback Method

Sources

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=C1118612&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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