«beta»-Aminobutyronitrile

Inchi:	InChI=1S/C4H8N2/c1-4(6)2-3-5/h4H,2,6H2,1H3
InchiKey:	PPBSMPOYVPZOFM-UHFFFAOYSA-N
Formula:	C4H8N2
SMILES:	CC(N)CC#N
Mol. weight [g/mol]:	84.12
CAS:	16750-40-6

Physical Properties

Property code	Value	Unit	Source
gf	179.99	kJ/mol	Joback Method
hf	67.50	kJ/mol	Joback Method
hfus	9.30	kJ/mol	Joback Method
hvap	45.23	kJ/mol	Joback Method
log10ws	-0.91		Crippen Method
logp	0.247		Crippen Method
mcvol	78.580	ml/mol	McGowan Method
pc	4098.62	kPa	Joback Method
tb	465.09	K	Joback Method
tc	676.22	K	Joback Method
tf	268.09	K	Joback Method
vc	0.308	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	159.57	J/mol×K	465.09	Joback Method
cpg	167.05	J/mol×K	500.28	Joback Method
cpg	174.17	J/mol×K	535.47	Joback Method
cpg	180.93	J/mol×K	570.65	Joback Method
cpg	187.34	J/mol×K	605.84	Joback Method
cpg	193.42	J/mol×K	641.03	Joback Method
cpg	199.17	J/mol×K	676.22	Joback Method

Sources

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=C16750406&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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