Cyclobutylamine

Other names:	Aminocyclobutane
	Cyclobutanamine
Inchi:	InChI=1S/C4H9N/c5-4-2-1-3-4/h4H,1-3,5H2
InchiKey:	KZZKOVLJUKWSKX-UHFFFAOYSA-N
Formula:	C4H9N
SMILES:	NC1CCC1
Mol. weight [g/mol]:	71.12
CAS:	2516-34-9

Physical Properties

Property code	Value	Unit	Source
chl	-2865.90 ± 0.54	kJ/mol	NIST Webbook
gf	97.90	kJ/mol	Joback Method
hf	41.00 ± 0.40	kJ/mol	NIST Webbook
hfl	5.61 ± 0.59	kJ/mol	NIST Webbook
hfus	7.35	kJ/mol	Joback Method
hvap	35.40	kJ/mol	NIST Webbook
hvap	36.00 ± 0.40	kJ/mol	NIST Webbook
ie	8.75 ± 0.03	eV	NIST Webbook
ie	8.60 ± 0.03	eV	NIST Webbook
log10ws	-0.94		Crippen Method
logp	0.498		Crippen Method
mcvol	66.340	ml/mol	McGowan Method
pc	5175.72	kPa	Joback Method
tb	355.20	K	NIST Webbook
tb	355.00	K	NIST Webbook
tc	581.69	K	Joback Method
tf	232.52	K	Joback Method
vc	0.237	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	118.69	J/mol×K	374.46	Joback Method

cpg	129.70	J/mol×K	409.00	Joback Method
cpg	140.07	J/mol×K	443.54	Joback Method
cpg	149.84	J/mol×K	478.07	Joback Method
cpg	159.02	J/mol×K	512.61	Joback Method
cpg	167.65	J/mol×K	547.15	Joback Method
cpg	175.75	J/mol×K	581.69	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	354.70	K	100.00	NIST Webbook

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=C2516349&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ie: Ionization energy
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

tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume