

CYCLOBUTYLAMINE

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

Physical Properties

Property code	Value	Unit	Source
chl	-2865.90 ± 0.54	kJ/mol	NIST Webbook
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	36.00 ± 0.40	kJ/mol	NIST Webbook
hvap	35.40	kJ/mol	NIST Webbook
ie	8.75 ± 0.03	eV	NIST Webbook
ie	8.60 ± 0.03	eV	NIST Webbook
logp	0.498		Crippen Method
mcvol	66.340	ml/mol	McGowan Method
tb	355.20	K	NIST Webbook
tb	355.00	K	NIST Webbook
tc	559.58	K	Cheméo Relay (1.0)
tf	183.96	K	Cheméo Relay (1.0)

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
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Pressure Dependent Properties

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

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C2516349&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
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
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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