1,4-Cyclohexanediamine

Other names:	1,4-Diaminocyclohexane
	cyclohexane-1,4-diamine
	TRANS-1,4-CYCLOHEXANEDIAMINE
Inchi:	InChI=1S/C6H14N2/c7-5-1-2-6(8)4-3-5/h5-6H,1-4,7-8H2
InchiKey:	VKIRRGRTJUUZHS-UHFFFAOYSA-N
Formula:	C6H14N2
SMILES:	NC1CCC(N)CC1
Mol. weight [g/mol]:	114.19
CAS:	3114-70-3

Physical Properties

Property code	Value	Unit	Source
hf	-68.21	kJ/mol	Cheméo Relay (1.0)
hfus	14.60	kJ/mol	Joback Method
hvap	60.13	kJ/mol	Cheméo Relay (1.0)
ie	8.40	eV	Cheméo Relay (1.0)
logp	0.215		Crippen Method
mcvol	104.500	ml/mol	McGowan Method
tb	454.20	K	NIST Webbook
tc	660.92	K	Cheméo Relay (1.0)
tf	311.16	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	48.20	kJ/mol	428.00	NIST Webbook

Correlations

Information	Value
Property code	cpg

Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-4.92500e+01
Coeff. B	7.93200e-01
Coeff. C	-4.15000e-04
Coeff. D	6.36000e-08
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3114703&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):
Cheméo Relay (1.0, beta):

Legend

cpg: Ideal gas heat capacity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
hvapt: Enthalpy of vaporization at a given temperature
ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

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