trans-1,4-Cyclohexanediamine

Other names:	1,4-Diaminocyclohexane
	1,4-Cyclohexanediamine
	cyclohexane-1,4-diamine
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
gf	149.28	kJ/mol	Joback Method
hf	-65.61	kJ/mol	Joback Method
hfus	14.60	kJ/mol	Joback Method
hvap	50.35	kJ/mol	Joback Method
log10ws	-1.32		Crippen Method
logp	0.215		Crippen Method
mcvol	104.500	ml/mol	McGowan Method
pc	4397.41	kPa	Joback Method
tb	454.20	K	NIST Webbook
tc	730.03	K	Joback Method
tf	327.04	K	Joback Method
vc	0.361	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.72	J/mol×K	691.13	Joback Method
cpg	250.11	J/mol×K	496.62	Joback Method
cpg	266.28	J/mol×K	535.52	Joback Method
cpg	281.50	J/mol×K	574.42	Joback Method
cpg	295.80	J/mol×K	613.32	Joback Method
cpg	309.20	J/mol×K	652.22	Joback Method

cpg	333.38	J/mol×K	730.03	Joback Method
hvapt	48.20	kJ/mol	428.00	NIST Webbook

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=C3114703&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
hvapt:	Enthalpy of vaporization at a given temperature
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