Cyclohexanamine, N-cyclohexyl-

Other names:	Aminodicyclohexane
	Bis(cyclohexyl)amine
	Cyclohexylcyclohexanamine
	DCH
	DCHA
	DODECAHYDRODIPHENYLAMINE
	Dicha
	Dicyclohexylamine
	Dicyklohexylamin
	N,N-Diclohexylamine
	N,N-Dicyclohexylamine
	N-CYCLOHEXYLCYCLOHEXANAMINE
	N-Cyclohexyl-cyclohexylamine
	NSC 3399
	UN 2565
Inchi:	InChI=1S/C12H23N/c1-3-7-11(8-4-1)13-12-9-5-2-6-10-12/h11-13H,1-10H2
InchiKey:	XBPCUCUWBYBCDP-UHFFFAOYSA-N
Formula:	C12H23N
SMILES:	C1CCC(NC2CCCCC2)CC1
Mol. weight [g/mol]:	181.32
CAS:	101-83-7

Physical Properties

Property code	Value	Unit	Source
chl	-7782.40 ± 2.70	kJ/mol	NIST Webbook
gf	188.45	kJ/mol	Joback Method
hf	-128.90	kJ/mol	Joback Method
hfl	-226.80 ± 2.70	kJ/mol	NIST Webbook
hfus	15.60	kJ/mol	Joback Method
hvap	49.60	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.241		Crippen Method
mcvol	168.200	ml/mol	McGowan Method
nfpaf	%!d(float64=1)		KDB
nfpah	%!d(float64=3)		KDB
pc	2637.96	kPa	Joback Method
rinpol	1408.00		NIST Webbook

rinpol	1431.48		NIST Webbook
rinpol	1392.00		NIST Webbook
rinpol	1392.00		NIST Webbook
rinpol	1444.00		NIST Webbook
rinpol	1442.00		NIST Webbook
rinpol	1437.00		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1437.00		NIST Webbook
ripol	1663.00		NIST Webbook
ripol	1673.00		NIST Webbook
ripol	1663.00		NIST Webbook
ripol	1683.00		NIST Webbook
tb	529.20	K	NIST Webbook
tb	524.65 ± 1.50	K	NIST Webbook
tb	522.15 ± 6.00	K	NIST Webbook
tc	794.59	K	Joback Method
tf	292.42	K	Joback Method
vc	0.609	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.72	J/mol×K	563.23	Joback Method
cpg	471.79	J/mol×K	601.79	Joback Method
cpg	495.24	J/mol×K	640.35	Joback Method
cpg	517.11	J/mol×K	678.91	Joback Method
cpg	537.46	J/mol×K	717.47	Joback Method
cpg	556.34	J/mol×K	756.03	Joback Method
cpg	573.82	J/mol×K	794.59	Joback Method
hvapt	54.00	kJ/mol	468.50	NIST Webbook
pvap	0.06	kPa	333.20	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	4.16e-03	kPa	298.30	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	5.50e-03	kPa	301.20	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study

pvap	7.06e-03	kPa	304.20	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	8.89e-03	kPa	307.20	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	0.01	kPa	310.20	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	0.01	kPa	313.20	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	3.22e-03	kPa	295.40	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	0.02	kPa	318.30	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	0.03	kPa	321.20	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	0.03	kPa	324.20	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	0.04	kPa	327.20	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	0.05	kPa	330.20	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study
pvap	0.02	kPa	315.10	Thermodynamic properties of cyclohexanamines: Experimental and theoretical study

rfi	1.48636	288.15	Experimental Determination and Modeling of Densities and Refractive Indices of the Binary Systems Alcohol + Dicyclohexylamine at T = (288.15 to 323.15) K
rfi	1.48416	293.15	Experimental Determination and Modeling of Densities and Refractive Indices of the Binary Systems Alcohol + Dicyclohexylamine at T = (288.15 to 323.15) K
rfi	1.48198	298.15	Experimental Determination and Modeling of Densities and Refractive Indices of the Binary Systems Alcohol + Dicyclohexylamine at T = (288.15 to 323.15) K
rfi	1.47978	303.15	Experimental Determination and Modeling of Densities and Refractive Indices of the Binary Systems Alcohol + Dicyclohexylamine at T = (288.15 to 323.15) K
rfi	1.47761	308.15	Experimental Determination and Modeling of Densities and Refractive Indices of the Binary Systems Alcohol + Dicyclohexylamine at T = (288.15 to 323.15) K

rfi	1.47562	313.15	Experimental Determination and Modeling of Densities and Refractive Indices of the Binary Systems Alcohol + Dicyclohexylamine at T = (288.15 to 323.15) K
rfi	1.47347	318.15	Experimental Determination and Modeling of Densities and Refractive Indices of the Binary Systems Alcohol + Dicyclohexylamine at T = (288.15 to 323.15) K
rfi	1.47134	323.15	Experimental Determination and Modeling of Densities and Refractive Indices of the Binary Systems Alcohol + Dicyclohexylamine at T = (288.15 to 323.15) K

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51017e+01
Coeff. B	-4.94503e+03
Coeff. C	-5.74970e+01
Temperature range (K), min.	391.30
Temperature range (K), max.	562.60

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.52535e+02
Coeff. B	-1.33522e+04

Coeff. C	-2.00181e+01
Coeff. D	1.01790e-05
Temperature range (K), min.	273.05
Temperature range (K), max.	737.00

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Experimental Determination and Modeling of Densities and Refractive Indices of the Binary Systems Alcohol + Isohexylamine at T = (288.15 to 323.15) K:	https://www.doi.org/10.1016/j.tca.2011.08.002
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1333
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Thermodynamic properties of cyclohexanamines: Experimental and theoretical study:	https://www.doi.org/10.1016/j.tca.2015.03.016
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C101837&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1333.mol
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume