1-Hexanamine

Other names:	1-AMINOHEXANE
	1-Hexylamine
	HEXYLAMINE
	Mono-n-hexylamine
	n-C6H13NH2
	n-Hexylamine
Inchi:	InChI=1S/C6H15N/c1-2-3-4-5-6-7/h2-7H2,1H3
InchiKey:	BMVXCPBXGZKUPN-UHFFFAOYSA-N
Formula:	C6H15N
SMILES:	CCCCCCN
Mol. weight [g/mol]:	101.19
CAS:	111-26-2

Physical Properties

Property code	Value	Unit	Source
affp	927.60	kJ/mol	NIST Webbook
affp	927.60	kJ/mol	NIST Webbook
affp	927.50	kJ/mol	NIST Webbook
basg	893.50	kJ/mol	NIST Webbook
chl	-4292.80	kJ/mol	NIST Webbook
gf	66.09	kJ/mol	Joback Method
hf	-193.90	kJ/mol	NIST Webbook
hfl	-239.00	kJ/mol	NIST Webbook
hfus	16.49	kJ/mol	Joback Method
hvap	45.00	kJ/mol	NIST Webbook
hvap	45.10 ± 0.10	kJ/mol	NIST Webbook
hvap	45.13	kJ/mol	NIST Webbook
hvap	45.10 ± 0.06	kJ/mol	NIST Webbook
ie	8.60	eV	NIST Webbook
ie	8.60	eV	NIST Webbook
ie	8.63 ± 0.05	eV	NIST Webbook
log10ws	-1.10		Aqueous Solubility Prediction Method
logp	1.525		Crippen Method
mcvol	105.380	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=2)		KDB

pc	3314.37	kPa	Joback Method
rinpol	835.30		NIST Webbook
rinpol	813.40		NIST Webbook
rinpol	816.00		NIST Webbook
rinpol	829.00		NIST Webbook
rinpol	848.00		NIST Webbook
rinpol	848.00		NIST Webbook
rinpol	839.00		NIST Webbook
rinpol	827.00		NIST Webbook
rinpol	834.40		NIST Webbook
rinpol	830.00		NIST Webbook
rinpol	829.00		NIST Webbook
rinpol	835.00		NIST Webbook
rinpol	831.00		NIST Webbook
rinpol	832.00		NIST Webbook
rinpol	813.40		NIST Webbook
rinpol	830.00		NIST Webbook
rinpol	839.00		NIST Webbook
rinpol	818.00		NIST Webbook
rinpol	830.00		NIST Webbook
rinpol	833.00		NIST Webbook
rinpol	830.00		NIST Webbook
ripol	1112.00		NIST Webbook
ripol	1115.00		NIST Webbook
ripol	1112.00		NIST Webbook
ripol	1113.00		NIST Webbook
ripol	1110.00		NIST Webbook
ripol	1123.00		NIST Webbook
ripol	1120.00		NIST Webbook
ripol	1115.00		NIST Webbook
tb	403.15	K	KDB
tc	592.30	K	Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons
tf	251.85	K	NIST Webbook
tf	251.17	K	Aqueous Solubility Prediction Method
tf	251.90 ± 0.60	K	NIST Webbook
tf	254.15 ± 2.00	K	NIST Webbook
tf	254.15 ± 1.00	K	NIST Webbook
tf	260.15 ± 4.00	K	NIST Webbook
vc	0.401	m3/kmol	Joback Method

volm	1.33e-04	m3/mol	Thermodynamic study of (heptane + amine) mixtures. II. Excess and partial molar volumes at 298.15 K

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	211.01	J/mol×K	409.21	Joback Method
cpg	263.66	J/mol×K	559.15	Joback Method
cpg	253.99	J/mol×K	529.16	Joback Method
cpg	243.90	J/mol×K	499.18	Joback Method
cpg	233.38	J/mol×K	469.19	Joback Method
cpg	222.42	J/mol×K	439.20	Joback Method
cpg	272.92	J/mol×K	589.14	Joback Method
cpl	252.00	J/mol×K	298.15	NIST Webbook
hvapt	42.20	kJ/mol	354.50	NIST Webbook
hvapt	36.54	kJ/mol	405.90	NIST Webbook
rhol	760.07	kg/m3	298.15	Thermodynamics of amide + amine mixtures. 1. Volumetric, speed of sound, and refractive index data for N,Ndimethylformamide + N-propylpropan-1-amine, + N-butylbutan-1-amine, + butan-1-amine, or + hexan-1-amine systems at several temperatures

rhol	764.42	kg/m3	293.15	Thermodynamics of amide + amine mixtures. 1. Volumetric, speed of sound, and refractive index data for N,Ndimethylformamide + N-propylpropan-1-amine, + N-butylbutan-1-amine, + butan-1-amine, or + hexan-1-amine systems at several temperatures
rhol	760.16	kg/m3	298.15	Thermodynamics of amide + amine mixtures. 5. Excess molar enthalpies of N,N-dimethylformamide or N,N-dimethylacetamide + N-propylpropan-1-amine, + N-butylbutan-1-amine, + butan-1-amine, or + hexan-1-amine systems at 298.15 K. Application of the ERAS model
rhol	755.85	kg/m3	303.15	Thermodynamics of amide + amine mixtures. 1. Volumetric, speed of sound, and refractive index data for N,Ndimethylformamide + N-propylpropan-1-amine, + N-butylbutan-1-amine, + butan-1-amine, or + hexan-1-amine systems at several temperatures

Correlations

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51494e+01
Coeff. B	-3.70763e+03
Coeff. C	-5.09360e+01
Temperature range (K), min.	300.41
Temperature range (K), max.	427.81

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.12428e+01
Coeff. B	-8.22951e+03
Coeff. C	-1.12604e+01
Coeff. D	7.80800e-06
Temperature range (K), min.	251.85
Temperature range (K), max.	583.00

Datasets

Viscosity, Pa*s

Pressure, kPa - Liquid	Temperature, K - Liquid	Viscosity, Pa*s - Liquid
100.00	293.15	0.0008380
100.00	313.15	0.0006180
100.00	333.15	0.0004800
100.00	353.15	0.0003840
20000.00	293.15	0.0009930
20000.00	313.15	0.0007240
20000.00	333.15	0.0005640
20000.00	353.15	0.0004550
40000.00	293.15	0.0011650
40000.00	313.15	0.0008480
40000.00	333.15	0.0006600
40000.00	353.15	0.0005330
60000.00	293.15	0.0013560
60000.00	313.15	0.0009860
60000.00	333.15	0.0007640

60000.00	353.15	0.0006130
80000.00	293.15	0.0015610
80000.00	313.15	0.0011380
80000.00	333.15	0.0008770
80000.00	353.15	0.0006970
100000.00	293.15	0.0017880
100000.00	313.15	0.0013040
100000.00	333.15	0.0009960
100000.00	353.15	0.0007830

Reference *https://www.doi.org/10.1016/j.jct.2008.08.006*

Mass density, kg/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m3 - Liquid
293.15	100.00	765.1
293.15	10000.00	771.5
293.15	20000.00	777.6
293.15	30000.00	783.4
293.15	40000.00	788.8
293.15	50000.00	793.8
293.15	60000.00	798.8
293.15	70000.00	803.3
293.15	80000.00	807.7
293.15	90000.00	811.9
293.15	100000.00	815.9
293.15	110000.00	819.8
293.15	120000.00	823.5
293.15	130000.00	827.1
293.15	140000.00	830.5
303.15	100.00	756.2
303.15	10000.00	763.5
303.15	20000.00	770.2
303.15	30000.00	776.3
303.15	40000.00	781.9
303.15	50000.00	787.2
303.15	60000.00	792.2
303.15	70000.00	796.9
303.15	80000.00	801.5
303.15	90000.00	805.8
303.15	100000.00	810.0

303.15	110000.00	814.0
303.15	120000.00	817.9
303.15	130000.00	821.6
303.15	140000.00	825.1
313.15	100.00	748.2
313.15	10000.00	755.4
313.15	20000.00	762.3
313.15	30000.00	768.6
313.15	40000.00	774.6
313.15	50000.00	780.2
313.15	60000.00	785.3
313.15	70000.00	790.3
313.15	80000.00	794.9
313.15	90000.00	799.4
313.15	100000.00	803.7
313.15	110000.00	807.8
313.15	120000.00	811.7
313.15	130000.00	815.5
313.15	140000.00	819.1
323.15	100.00	738.9
323.15	10000.00	746.9
323.15	20000.00	754.2
323.15	30000.00	761.0
323.15	40000.00	767.2
323.15	50000.00	772.9
323.15	60000.00	778.4
323.15	70000.00	783.5
323.15	80000.00	788.4
323.15	90000.00	792.9
323.15	100000.00	797.3
323.15	110000.00	801.7
323.15	120000.00	805.8
323.15	130000.00	809.7
323.15	140000.00	813.5
333.15	100.00	730.2
333.15	10000.00	738.7
333.15	20000.00	746.3
333.15	30000.00	753.4
333.15	40000.00	759.9
333.15	50000.00	765.9
333.15	60000.00	771.6
333.15	70000.00	776.9
333.15	80000.00	781.9
333.15	90000.00	786.7

333.15	100000.00	791.2
333.15	110000.00	795.7
333.15	120000.00	799.9
333.15	130000.00	803.8
333.15	140000.00	807.6
343.15	100.00	721.3
343.15	10000.00	730.6
343.15	20000.00	738.8
343.15	30000.00	746.4
343.15	40000.00	753.2
343.15	50000.00	759.6
343.15	60000.00	765.6
343.15	70000.00	771.0
343.15	80000.00	776.2
343.15	90000.00	781.1
343.15	100000.00	785.9
343.15	110000.00	790.3
343.15	120000.00	794.6
343.15	130000.00	798.8
343.15	140000.00	802.7
353.15	100.00	712.4
353.15	10000.00	722.3
353.15	20000.00	731.1
353.15	30000.00	739.0
353.15	40000.00	746.0
353.15	50000.00	752.5
353.15	60000.00	759.0
353.15	70000.00	764.6
353.15	80000.00	770.0
353.15	90000.00	775.1
353.15	100000.00	780.0
353.15	110000.00	784.6
353.15	120000.00	789.1
353.15	130000.00	793.2
353.15	140000.00	797.3

Reference *https://www.doi.org/10.1016/j.jct.2008.01.006*

Temperature, K	Pressure, kPa	Mass density, kg/m3
293.15	100.00	765.0
293.15	10000.00	771.2
293.15	20000.00	777.4
293.15	30000.00	783.2

293.15	40000.00	788.6
293.15	50000.00	793.7
293.15	60000.00	798.6
293.15	70000.00	803.1
293.15	80000.00	807.5
293.15	90000.00	811.8
293.15	100000.00	815.8
293.15	110000.00	819.6
293.15	120000.00	823.3
293.15	130000.00	826.9
293.15	140000.00	830.3
353.15	100.00	712.4
353.15	10000.00	722.4
353.15	20000.00	731.1
353.15	30000.00	739.1
353.15	40000.00	746.2
353.15	50000.00	752.8
353.15	60000.00	758.9
353.15	70000.00	764.7
353.15	80000.00	770.1
353.15	90000.00	775.2
353.15	100000.00	780.1
353.15	110000.00	784.7
353.15	120000.00	789.2
353.15	130000.00	793.4
353.15	140000.00	797.5
363.15	100.00	703.9
363.15	10000.00	714.4
363.15	20000.00	723.6
363.15	30000.00	731.9
363.15	40000.00	739.3
363.15	50000.00	746.2
363.15	60000.00	752.6
363.15	70000.00	758.5
363.15	80000.00	764.1
363.15	90000.00	769.4
363.15	100000.00	774.4
363.15	110000.00	779.1
363.15	120000.00	783.6
363.15	130000.00	787.9
363.15	140000.00	792.1
373.15	100.00	694.8
373.15	10000.00	706.0
373.15	20000.00	716.0

373.15	30000.00	724.5
373.15	40000.00	732.4
373.15	50000.00	739.5
373.15	60000.00	746.1
373.15	70000.00	752.2
373.15	80000.00	758.1
373.15	90000.00	763.5
373.15	100000.00	768.7
373.15	110000.00	773.5
373.15	120000.00	778.2
373.15	130000.00	782.6
373.15	140000.00	786.9
383.15	100.00	686.1
383.15	10000.00	698.2
383.15	20000.00	708.6
383.15	30000.00	717.6
383.15	40000.00	725.8
383.15	50000.00	733.3
383.15	60000.00	740.2
383.15	70000.00	746.5
383.15	80000.00	752.5
383.15	90000.00	758.1
383.15	100000.00	763.4
383.15	110000.00	768.3
383.15	120000.00	773.2
383.15	130000.00	777.7
383.15	140000.00	782.0
393.15	100.00	676.2
393.15	10000.00	689.2
393.15	20000.00	700.3
393.15	30000.00	709.8
393.15	40000.00	718.4
393.15	50000.00	726.6
393.15	60000.00	733.7
393.15	70000.00	740.3
393.15	80000.00	746.5
393.15	90000.00	752.2
393.15	100000.00	757.7
393.15	110000.00	762.9
393.15	120000.00	767.8
393.15	130000.00	772.5
393.15	140000.00	776.9
403.15	100.00	666.9
403.15	10000.00	680.9

403.15	20000.00	692.5
403.15	30000.00	702.8
403.15	40000.00	711.7
403.15	50000.00	719.9
403.15	60000.00	727.2
403.15	70000.00	734.1
403.15	80000.00	740.4
403.15	90000.00	746.5
403.15	100000.00	752.1
403.15	110000.00	757.4
403.15	120000.00	762.5
403.15	130000.00	767.2
403.15	140000.00	771.8

Reference *https://www.doi.org/10.1016/j.jct.2012.09.016*

Sources

Thermodynamic study of (heptane + amine) mixtures. II. Excess and partial molar volumes at 298.15 K:	https://www.doi.org/10.1016/j.jct.2010.12.025
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Pure (Korean Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1269
Heat capacity of 1-pentylamine and 1-hexylamine: Experimental determination and modeling through a cubic-state association model (TSAM):	https://www.doi.org/10.1016/j.jct.2012.09.016
Thermodynamic study of heptane + amine mixtures. V. Excess and solvation Gibbs energies:	https://www.doi.org/10.1016/j.fluid.2014.12.017
Thermodynamics of amide + amine mixtures. 5. Excess molar enthalpies of N,N-dimethylformamide or N,N-dimeth Pacetamide, + N-propylpropan-1-amine, + N-butylbutan-1-amine, or + hexan-1-amine systems at 298.15 K:	https://www.doi.org/10.1016/j.fluid.2019.112283
Thermodynamics of amide + amine mixtures. I. Volumetric, speed of sound and isentropic data for N,N-dimethylformamide + butan-1-amine, or + hexan-1-amine systems at 298.15 K:	https://www.doi.org/10.1021/acs.jced.5b00802
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1269
NIST Webbook: 1-amine, N-butylbutan-1-amine + butan-1-amine, or + hexan-1-amine systems at several temperatures:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C111262&Units=SI
KDB Application of the ERAS model:	https://www.cheric.org/files/research/kdb/mol/mol1269.mol
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Influence of the chain length on the dynamic viscosity at high pressure of some amines: Measurements and correlative study of some models:	https://www.doi.org/10.1016/j.jct.2008.08.006
Gas-Liquid Critical Temperatures of Some Alkanes, Amines, and Cyclic Hydrocarbons:	https://www.doi.org/10.1021/je0341357
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Thermodynamic Parameters of Anionic Surfactant-Additive Systems at the Cloud Point:	https://www.doi.org/10.1021/je100502b
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
1-Butanol + hexylamine + n-heptane at temperature range (288.15 323.15 K):	https://www.doi.org/10.1016/j.fluid.2010.07.011
High-pressure (up to 140 MPa) density and derivative properties of some (normal-hexyl- and heptyl-) amines between (293.15 and 353.15) K:	https://www.doi.org/10.1016/j.jct.2008.01.006
Experimental density data, excess molar volumes determination and modeling with cubic EoSs:	

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
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
ie:	Ionization energy
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
rhol:	Liquid Density
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
volm:	Molar Volume