1-Heptanamine

Other names:	1-AMINOHEPTANE
	1-Heptylamine
	CH3(CH2)6NH2
	HEPTYLAMINE
	N-HEPTYLAMINE
Inchi:	InChI=1S/C7H17N/c1-2-3-4-5-6-7-8/h2-8H2,1H3
InchiKey:	WJYIASZWHGOTOU-UHFFFAOYSA-N
Formula:	C7H17N
SMILES:	CCCCCCCN
Mol. weight [g/mol]:	115.22
CAS:	111-68-2

Physical Properties

Property code	Value	Unit	Source
affp	923.20	kJ/mol	NIST Webbook
basg	879.50 ± 9.20	kJ/mol	NIST Webbook
basg	889.30	kJ/mol	NIST Webbook
chl	-4949.70	kJ/mol	NIST Webbook
gf	74.51	kJ/mol	Joback Method
hf	-216.00	kJ/mol	NIST Webbook
hfl	-266.00	kJ/mol	NIST Webbook
hfus	19.08	kJ/mol	Joback Method
hvap	50.00 ± 0.10	kJ/mol	NIST Webbook
hvap	49.90	kJ/mol	NIST Webbook
hvap	49.96 ± 0.08	kJ/mol	NIST Webbook
hvap	49.98	kJ/mol	NIST Webbook
log10ws	-1.85		Aqueous Solubility Prediction Method
logp	1.915		Crippen Method
mcvol	119.470	ml/mol	McGowan Method
pc	2976.29	kPa	Joback Method
rinpol	931.00		NIST Webbook
rinpol	935.00		NIST Webbook
rinpol	930.00		NIST Webbook
rinpol	931.00		NIST Webbook
rinpol	932.00		NIST Webbook
rinpol	932.00		NIST Webbook

rinpol	932.00		NIST Webbook
rinpol	933.00		NIST Webbook
rinpol	933.00		NIST Webbook
rinpol	934.00		NIST Webbook
rinpol	932.00		NIST Webbook
rinpol	933.00		NIST Webbook
rinpol	933.00		NIST Webbook
rinpol	934.00		NIST Webbook
rinpol	935.00		NIST Webbook
rinpol	939.00		NIST Webbook
rinpol	931.00		NIST Webbook
rinpol	933.00		NIST Webbook
rinpol	930.00		NIST Webbook
rinpol	942.00		NIST Webbook
rinpol	912.00		NIST Webbook
rinpol	930.00		NIST Webbook
rinpol	937.00		NIST Webbook
rinpol	941.00		NIST Webbook
rinpol	933.00		NIST Webbook
rinpol	934.00		NIST Webbook
rinpol	935.00		NIST Webbook
rinpol	932.00		NIST Webbook
rinpol	933.00		NIST Webbook
rinpol	932.00		NIST Webbook
rinpol	932.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	943.20		NIST Webbook
rinpol	928.00		NIST Webbook
rinpol	942.00		NIST Webbook
rinpol	931.00		NIST Webbook
rinpol	934.00		NIST Webbook
ripol	1215.00		NIST Webbook
ripol	1218.00		NIST Webbook
ripol	1213.00		NIST Webbook
ripol	1215.00		NIST Webbook
ripol	1223.00		NIST Webbook
ripol	1219.00		NIST Webbook
ripol	1220.00		NIST Webbook
ripol	1217.00		NIST Webbook
tb	432.09	K	Joback Method
tc	610.78	K	Joback Method
tf	253.48	K	Aqueous Solubility Prediction Method
tf	250.15 ± 0.60	K	NIST Webbook
vc	0.457	m3/kmol	Joback Method

volm	1.50e-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	263.29	J/mol×K	461.87	Joback Method
cpg	318.89	J/mol×K	610.78	Joback Method
cpg	308.70	J/mol×K	581.00	Joback Method
cpg	298.06	J/mol×K	551.21	Joback Method
cpg	286.95	J/mol×K	521.43	Joback Method
cpg	275.37	J/mol×K	491.65	Joback Method
cpg	250.70	J/mol×K	432.09	Joback Method
hvapt	46.50	kJ/mol	378.00	NIST Webbook
pvap	0.38	kPa	302.20	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration
pvap	0.29	kPa	298.30	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration

pvap	0.33	kPa	300.30	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	
pvap	0.25	kPa	296.20	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	
pvap	0.41	kPa	303.20	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	
pvap	0.50	kPa	306.20	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	

pvap	0.22	kPa	294.20	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration
pvap	0.19	kPa	292.20	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration
pvap	0.16	kPa	290.20	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration
pvap	0.14	kPa	288.20	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration

pvap	0.12	kPa	286.20	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration
pvap	0.11	kPa	284.20	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration
pvap	0.09	kPa	282.20	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration
pvap	0.08	kPa	280.20	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.57790e+01
Coeff. B	-4.11042e+03
Coeff. C	-6.07040e+01
Temperature range (K), min.	326.04
Temperature range (K), max.	453.39

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.39695e+02
Coeff. B	-1.08451e+04
Coeff. C	-1.85086e+01
Coeff. D	1.28802e-05
Temperature range (K), min.	254.15
Temperature range (K), max.	607.00

Datasets

Viscosity, Pa*s

Pressure, kPa - Liquid	Temperature, K - Liquid	Viscosity, Pa*s - Liquid
100.00	293.15	0.0010780
100.00	313.15	0.0007870
100.00	333.15	0.0006050
100.00	353.15	0.0004640
20000.00	293.15	0.0012890
20000.00	313.15	0.0009050
20000.00	333.15	0.0007000
20000.00	353.15	0.0005520
40000.00	293.15	0.0015220
40000.00	313.15	0.0010650
40000.00	333.15	0.0008230
40000.00	353.15	0.0006510
60000.00	293.15	0.0017870

60000.00	313.15	0.0012500
60000.00	333.15	0.0009530
60000.00	353.15	0.0007540
80000.00	293.15	0.0020740
80000.00	313.15	0.0014600
80000.00	333.15	0.0010940
80000.00	353.15	0.0008620
100000.00	293.15	0.0023990
100000.00	313.15	0.0016980
100000.00	333.15	0.0012430
100000.00	353.15	0.0009760

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	774.9
293.15	10000.00	781.1
293.15	20000.00	787.1
293.15	30000.00	792.6
293.15	40000.00	797.8
293.15	50000.00	802.7
293.15	60000.00	807.4
293.15	70000.00	811.8
293.15	80000.00	816.1
293.15	90000.00	820.2
293.15	100000.00	824.0
293.15	110000.00	827.8
293.15	120000.00	831.5
293.15	130000.00	835.0
293.15	140000.00	838.3
303.15	100.00	766.5
303.15	10000.00	773.6
303.15	20000.00	780.0
303.15	30000.00	785.8
303.15	40000.00	791.3
303.15	50000.00	796.5
303.15	60000.00	801.3
303.15	70000.00	806.0
303.15	80000.00	810.4

303.15	90000.00	814.6
303.15	100000.00	818.7
303.15	110000.00	822.5
303.15	120000.00	826.2
303.15	130000.00	829.9
303.15	140000.00	833.3
313.15	100.00	758.2
313.15	10000.00	765.4
313.15	20000.00	772.0
313.15	30000.00	778.2
313.15	40000.00	784.0
313.15	50000.00	789.3
313.15	60000.00	794.5
313.15	70000.00	799.2
313.15	80000.00	803.7
313.15	90000.00	808.0
313.15	100000.00	812.2
313.15	110000.00	816.2
313.15	120000.00	820.1
313.15	130000.00	823.8
313.15	140000.00	827.4
323.15	100.00	749.8
323.15	10000.00	757.6
323.15	20000.00	764.5
323.15	30000.00	771.0
323.15	40000.00	777.0
323.15	50000.00	782.6
323.15	60000.00	787.8
323.15	70000.00	792.7
323.15	80000.00	797.5
323.15	90000.00	802.0
323.15	100000.00	806.3
323.15	110000.00	810.6
323.15	120000.00	814.5
323.15	130000.00	818.4
323.15	140000.00	822.1
333.15	100.00	741.4
333.15	10000.00	749.5
333.15	20000.00	756.8
333.15	30000.00	763.4
333.15	40000.00	769.6
333.15	50000.00	775.5
333.15	60000.00	780.9
333.15	70000.00	786.2

333.15	80000.00	791.1
333.15	90000.00	795.6
333.15	100000.00	800.0
333.15	110000.00	804.3
333.15	120000.00	808.4
333.15	130000.00	812.4
333.15	140000.00	816.2
343.15	100.00	732.6
343.15	10000.00	741.7
343.15	20000.00	749.6
343.15	30000.00	756.7
343.15	40000.00	763.3
343.15	50000.00	769.4
343.15	60000.00	775.1
343.15	70000.00	780.4
343.15	80000.00	785.5
343.15	90000.00	790.3
343.15	100000.00	794.9
343.15	110000.00	799.2
343.15	120000.00	803.3
343.15	130000.00	807.4
343.15	140000.00	811.3
353.15	100.00	724.4
353.15	10000.00	733.7
353.15	20000.00	741.9
353.15	30000.00	749.3
353.15	40000.00	756.2
353.15	50000.00	762.6
353.15	60000.00	768.7
353.15	70000.00	774.2
353.15	80000.00	779.5
353.15	90000.00	784.3
353.15	100000.00	789.2
353.15	110000.00	793.7
353.15	120000.00	797.9
353.15	130000.00	802.1
353.15	140000.00	806.1

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

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
Grippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Thermodynamic Parameters of Anionic Surfactant-Additive Systems at the Cloud Point:	https://www.doi.org/10.1021/je100502b
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1477.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1477
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Stimulants at 298.15 K:	https://www.doi.org/10.1021/je400212t
Thermodynamic study of heptane + amine mixtures. V. Excess and partial molar volumes at 313.15 K:	https://www.doi.org/10.1016/j.fluid.2014.12.017
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C111682&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
High-pressure (up to 140 MPa) density and derivative properties of some (pentyl-, hexyl-, and heptyl-) amines between (293.15 and 353.15) K:	https://www.doi.org/10.1016/j.jct.2008.01.006
Influence of the chain length on the dynamic viscosity at high pressure of some amines: Measurements and comparative study of some models:	https://www.doi.org/10.1016/j.jct.2008.08.006

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas 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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
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