Heptane, 1-chloro-

Other names:	1-Chloroheptane
	Heptyl chloride
	N-HEPTYL CHLORIDE
Inchi:	InChI=1S/C7H15Cl/c1-2-3-4-5-6-7-8/h2-7H2,1H3
InchiKey:	DZMDPHNGKBEVRE-UHFFFAOYSA-N
Formula:	C7H15Cl
SMILES:	CCCCCCCCl
Mol. weight [g/mol]:	134.65
CAS:	629-06-1

Physical Properties

Property code	Value	Unit	Source
gf	-3.87	kJ/mol	Joback Method
hf	-203.55	kJ/mol	Joback Method
hfus	18.08	kJ/mol	Joback Method
hvap	47.00	kJ/mol	NIST Webbook
hvap	47.70 ± 0.10	kJ/mol	NIST Webbook
hvap	47.66 ± 0.10	kJ/mol	NIST Webbook
hvap	47.90	kJ/mol	NIST Webbook
hvap	47.68	kJ/mol	NIST Webbook
ie	10.15	eV	NIST Webbook
log10ws	-3.99		Aqueous Solubility Prediction Method
log10ws	-4.00		Estimated Solubility Method
logp	3.196		Crippen Method
mcvol	121.730	ml/mol	McGowan Method
pc	2693.00	kPa	Joback Method
rinpol	945.00		NIST Webbook
rinpol	958.00		NIST Webbook
rinpol	948.00		NIST Webbook
rinpol	962.00		NIST Webbook
rinpol	949.00		NIST Webbook
rinpol	945.00		NIST Webbook
rinpol	958.00		NIST Webbook
rinpol	934.50		NIST Webbook
rinpol	948.30		NIST Webbook
rinpol	945.00		NIST Webbook

ripol	1151.00		NIST Webbook
ripol	1150.00		NIST Webbook
ripol	1135.00		NIST Webbook
ripol	1142.00		NIST Webbook
ripol	1154.00		NIST Webbook
ripol	1155.00		NIST Webbook
ripol	1152.00		NIST Webbook
tb	431.55 ± 1.00	K	NIST Webbook
tb	433.15	K	KDB
tb	432.20	K	NIST Webbook
tb	433.15 ± 0.30	K	NIST Webbook
tc	568.65	K	Joback Method
tf	203.65 ± 0.40	K	NIST Webbook
tf	203.40	K	Aqueous Solubility Prediction Method
vc	0.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.48	J/mol×K	568.65	Joback Method
cpg	234.85	J/mol×K	425.60	Joback Method
cpg	246.03	J/mol×K	454.21	Joback Method
cpg	256.77	J/mol×K	482.82	Joback Method
cpg	267.08	J/mol×K	511.43	Joback Method
cpg	276.99	J/mol×K	540.04	Joback Method
cpg	223.23	J/mol×K	396.99	Joback Method
cpl	247.03	J/mol×K	301.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis

cpl	247.61	J/mol×K	304.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	248.53	J/mol×K	306.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	249.54	J/mol×K	309.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	250.65	J/mol×K	311.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	

cpl	251.60	J/mol×K	314.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	252.20	J/mol×K	316.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	253.36	J/mol×K	319.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	254.42	J/mol×K	321.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	

cpl	254.76	J/mol×K	324.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	256.19	J/mol×K	326.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	246.05	J/mol×K	299.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	258.06	J/mol×K	331.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	

cpl	258.84	J/mol×K	334.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	259.88	J/mol×K	336.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	261.01	J/mol×K	339.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	261.55	J/mol×K	341.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	

cpl	262.90	J/mol×K	344.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	263.26	J/mol×K	346.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	264.30	J/mol×K	349.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	266.04	J/mol×K	351.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	

cpl	266.51	J/mol×K	353.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	245.40	J/mol×K	298.15	NIST Webbook	
cpl	245.23	J/mol×K	296.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	244.29	J/mol×K	294.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	243.40	J/mol×K	291.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	

cpl	242.67	J/mol×K	289.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	241.75	J/mol×K	286.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	257.57	J/mol×K	329.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
cpl	240.95	J/mol×K	284.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis	
dvisc	0.0007503	Pa×s	297.78	Joback Method	
dvisc	0.0005116	Pa×s	330.85	Joback Method	
dvisc	0.0003740	Pa×s	363.92	Joback Method	
dvisc	0.0050881	Pa×s	198.57	Joback Method	
dvisc	0.0022404	Pa×s	231.64	Joback Method	
dvisc	0.0012109	Pa×s	264.71	Joback Method	

dvisc	0.0002880	Pa×s	396.99	Joback Method
hvapt	45.10	kJ/mol	394.00	NIST Webbook
hvapt	46.90	kJ/mol	370.50	NIST Webbook
rfi	1.42360		298.15	Densities, Excess Molar Volumes, Viscosities, and Refractive Indices of Binary Mixtures of n-Butyl Acetate with 1-Chloroalkanes (C4 C8) at 298.15 K
rhol	830.60	kg/m3	343.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K
rhol	812.60	kg/m3	363.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K
rhol	848.20	kg/m3	323.65	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K
rhol	870.40	kg/m3	298.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K
rhol	874.50	kg/m3	293.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K
rhol	883.40	kg/m3	283.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K

rhol	891.70	kg/m3	273.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K
rhol	900.40	kg/m3	263.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K
rhol	908.30	kg/m3	253.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K
rhol	784.40	kg/m3	393.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54644e+01
Coeff. B	-4.02446e+03
Coeff. C	-6.11490e+01
Temperature range (K), min.	326.32
Temperature range (K), max.	457.53

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.30860e+02
Coeff. B	-1.03354e+04
Coeff. C	-1.72470e+01
Coeff. D	1.23476e-05
Temperature range (K), min.	307.15

Temperature range (K), max.	433.15

Sources

Does Alkyl Chain Length Really Matter? Structure-Property Relationships in Thermochemistry of Ionic Liquids.:	https://www.doi.org/10.1016/j.tca.2013.04.003
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1639
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Density of Some 1-Chloroalkanes within the Temperature Range from (283.15 to 423.15) K:	https://www.doi.org/10.1021/je700325c
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C629061&Units=SI
Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 333.15 K. A group additivity and molecular connectivity analysis:	https://www.doi.org/10.1021/je049652j
Densities, Excess Molar Volumes, Viscosities, and Refractive Indices of Binary Mixtures of n-Butyl Acetate with 1-Chloroalkanes (C4 C8) at 298.15 K:	https://www.doi.org/10.1007/s10765-010-0902-x
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1639.mol
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

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
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
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
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