Pentane, 1-chloro-

Other names:	1-Chloropentane
	Amyl chloride
	N-AMYL CHLORIDE
	N-PENTYL CHLORIDE
	Pentyl chloride
	UN 1107
Inchi:	InChI=1S/C5H11Cl/c1-2-3-4-5-6/h2-5H2,1H3
InchiKey:	SQCZQTSHSZLZIQ-UHFFFAOYSA-N
Formula:	C5H11Cl
SMILES:	CCCCCCl
Mol. weight [g/mol]:	106.59
CAS:	543-59-9

Physical Properties

Property code	Value	Unit	Source
af	0.4370		KDB
chl	-3344.60	kJ/mol	NIST Webbook
chl	-3352.00 ± 3.00	kJ/mol	NIST Webbook
chl	-3349.90 ± 1.20	kJ/mol	NIST Webbook
gf	-20.71	kJ/mol	Joback Method
hf	-175.20 ± 1.30	kJ/mol	NIST Webbook
hfl	-213.40 ± 1.30	kJ/mol	NIST Webbook
hfl	-212.00 ± 3.00	kJ/mol	NIST Webbook
hfus	12.90	kJ/mol	Joback Method
hvap	38.20 ± 0.10	kJ/mol	NIST Webbook
hvap	38.30	kJ/mol	NIST Webbook
hvap	38.24 ± 0.02	kJ/mol	NIST Webbook
hvap	38.21	kJ/mol	NIST Webbook
hvap	38.20	kJ/mol	NIST Webbook
hvap	38.80	kJ/mol	NIST Webbook
ie	10.47	eV	NIST Webbook
log10ws	-2.73		Aqueous Solubility Prediction Method
log10ws	-2.73		Estimated Solubility Method
logp	2.415		Crippen Method
mcvol	93.550	ml/mol	McGowan Method

nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=1)		KDB
pc	3320.00	kPa	KDB
rinpol	754.00		NIST Webbook
rinpol	725.00		NIST Webbook
rinpol	729.00		NIST Webbook
rinpol	730.00		NIST Webbook
rinpol	722.00		NIST Webbook
rinpol	756.00		NIST Webbook
rinpol	754.20		NIST Webbook
rinpol	736.00		NIST Webbook
rinpol	739.00		NIST Webbook
rinpol	747.00		NIST Webbook
rinpol	743.00		NIST Webbook
rinpol	744.00		NIST Webbook
rinpol	732.20		NIST Webbook
rinpol	746.00		NIST Webbook
rinpol	748.00		NIST Webbook
rinpol	751.00		NIST Webbook
rinpol	744.00		NIST Webbook
rinpol	742.00		NIST Webbook
rinpol	740.00		NIST Webbook
rinpol	751.10		NIST Webbook
rinpol	743.40		NIST Webbook
rinpol	742.00		NIST Webbook
rinpol	747.00		NIST Webbook
rinpol	748.00		NIST Webbook
rinpol	762.00		NIST Webbook
rinpol	722.00		NIST Webbook
rinpol	756.00		NIST Webbook
rinpol	742.00		NIST Webbook
rinpol	741.70		NIST Webbook
rinpol	742.20		NIST Webbook
rinpol	742.20		NIST Webbook
rinpol	762.00		NIST Webbook
ripol	941.00		NIST Webbook
ripol	945.00		NIST Webbook
ripol	943.00		NIST Webbook
ripol	953.00		NIST Webbook
ripol	946.00		NIST Webbook
ripol	938.00		NIST Webbook
ripol	945.00		NIST Webbook
ripol	945.00		NIST Webbook
ripol	938.00		NIST Webbook

tb	380.20	K	KDB
tc	552.00	K	KDB
tc	568.50	K	NIST Webbook
tf	174.00	K	KDB
vc	0.364	m3/kmol	KDB
zc	0.2636690		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	160.12	J/mol×K	379.98	Joback Method
cpg	177.07	J/mol×K	437.47	Joback Method
cpg	168.76	J/mol×K	408.72	Joback Method
cpg	200.12	J/mol×K	523.71	Joback Method
cpg	151.15	J/mol×K	351.23	Joback Method
cpg	185.06	J/mol×K	466.22	Joback Method
cpg	192.74	J/mol×K	494.97	Joback Method
cpl	190.99	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	189.81	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	190.32	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	189.19	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	191.89	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	192.65	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	193.22	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	188.46	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	194.69	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	195.06	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	196.14	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	196.99	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	197.64	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	198.46	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	187.66	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	199.92	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	200.41	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	201.19	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	201.73	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	202.54	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	203.57	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	204.24	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	187.70	J/mol×K	298.15	NIST Webbook	

cpl	194.09	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	187.16	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	186.52	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	185.95	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	185.29	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	199.23	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	184.57	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	0.0019882	Pa×s	205.23	Joback Method
dvisc	0.0003693	Pa×s	322.03	Joback Method
dvisc	0.0004960	Pa×s	292.83	Joback Method
dvisc	0.0007111	Pa×s	263.63	Joback Method
dvisc	0.0011153	Pa×s	234.43	Joback Method
dvisc	0.0042937	Pa×s	176.03	Joback Method
dvisc	0.0002888	Pa×s	351.23	Joback Method
hvapt	36.20	kJ/mol	303.00	NIST Webbook
hvapt	34.60	kJ/mol	358.00	NIST Webbook
hvapt	34.00	kJ/mol	363.00	NIST Webbook
hvapt	35.60	kJ/mol	343.00	NIST Webbook
hvapt	36.50	kJ/mol	328.00	NIST Webbook
hvapt	37.30	kJ/mol	313.00	NIST Webbook
hvapt	38.70	kJ/mol	349.00	NIST Webbook
hvapt	33.15	kJ/mol	380.90	NIST Webbook

hvapt	33.20	kJ/mol	378.00	NIST Webbook
hvapt	33.18	kJ/mol	380.20	KDB
kvisc	0.0000005	m2/s	313.15	Experimental and predicted viscosities of binary mixtures of cyclic ethers with 1-chloropentane or 1-chlorohexane at 283.15, 298.15, and 313.15K
kvisc	0.0000006	m2/s	298.15	Experimental and predicted viscosities of binary mixtures of cyclic ethers with 1-chloropentane or 1-chlorohexane at 283.15, 298.15, and 313.15K
kvisc	0.0000007	m2/s	283.15	Experimental and predicted viscosities of binary mixtures of cyclic ethers with 1-chloropentane or 1-chlorohexane at 283.15, 298.15, and 313.15K
pvap	8.45	kPa	313.15	Isothermal vapour-liquid equilibrium for cyclic ethers with 1-chloropentane
pvap	16.40	kPa	328.15	Isothermal vapour-liquid equilibrium for cyclic ethers with 1-chloropentane
pvap	4.05	kPa	298.15	Isothermal vapour-liquid equilibrium for cyclic ethers with 1-chloropentane

rfi	1.40970		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
rfi	1.41015		298.15	Isothermal vapor liquid equilibria and excess Gibbs free energies in some binary nitroalkane + chloroalkane mixtures at temperatures from 298.15 K to 318.15 K
rhol	851.30	kg/m3	323.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K
rhol	879.80	kg/m3	298.15	Volumetric and optical properties for some (2-butanone + chloroalkane) binary mixtures at T = 298.15 K
rhol	877.09	kg/m3	298.15	Volumetric Study for the Binary Nitromethane with Chloroalkane Mixtures at Temperatures in the Range (298.15 to 318.15) K
rhol	866.97	kg/m3	308.15	Volumetric Study for the Binary Nitromethane with Chloroalkane Mixtures at Temperatures in the Range (298.15 to 318.15) K

rhol	856.73	kg/m3	318.15	Volumetric Study for the Binary Nitromethane with Chloroalkane Mixtures at Temperatures in the Range (298.15 to 318.15) K
rhol	917.50	kg/m3	253.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K
rhol	910.20	kg/m3	263.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K
rhol	900.70	kg/m3	273.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K
rhol	891.00	kg/m3	283.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K
rhol	881.30	kg/m3	293.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K
rhol	809.10	kg/m3	363.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) 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	876.20	kg/m3	298.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K
speedsl	1085.84	m/s	318.15	Speeds of sound, isentropic compressibilities and refractive indices for some binary mixtures of nitromethane with chloroalkane at temperatures from 298.15 to 318.15 K. Comparison with theories
speedsl	1124.94	m/s	308.15	Speeds of sound, isentropic compressibilities and refractive indices for some binary mixtures of nitromethane with chloroalkane at temperatures from 298.15 to 318.15 K. Comparison with theories
speedsl	1164.24	m/s	298.15	Speeds of sound, isentropic compressibilities and refractive indices for some binary mixtures of nitromethane with chloroalkane at temperatures from 298.15 to 318.15 K. Comparison with theories
srf	0.02	N/m	298.15	Surface and bulk behaviour of some (n-hexane + chloroalkane) mixtures
srf	0.02	N/m	303.15	Surface and bulk behaviour of some (n-hexane + chloroalkane) mixtures
srf	0.02	N/m	308.15	Surface and bulk behaviour of some (n-hexane + chloroalkane) mixtures

srf	0.03	N/m	283.15	Surface and bulk behaviour of some (n-hexane + chloroalkane) mixtures
srf	0.03	N/m	288.15	Surface and bulk behaviour of some (n-hexane + chloroalkane) mixtures
srf	0.03	N/m	293.15	Surface and bulk behaviour of some (n-hexane + chloroalkane) mixtures
srf	0.02	N/m	313.15	Surface and bulk behaviour of some (n-hexane + chloroalkane) mixtures

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	278.20	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46439e+01
Coeff. B	-3.45471e+03
Coeff. C	-3.64100e+01
Temperature range (K), min.	277.05
Temperature range (K), max.	406.59

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.39136e+01
Coeff. B	-6.80056e+03

Coeff. C	-8.81199e+00
Coeff. D	6.28593e-06
Temperature range (K), min.	174.15
Temperature range (K), max.	588.00

Sources

Isothermal vapour-liquid equilibrium for cyclic ethers with 1-chloropentane:	https://www.doi.org/10.1016/j.fluid.2006.10.024
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1622.mol
Surface and bulk behaviour of some (n-hexane + chloroalkane) mixtures:	https://www.doi.org/10.1016/j.jct.2008.10.016
Activity Coefficients at Infinite Dilution by GLC in Alkanediamines as Stationary Phases:	https://www.doi.org/10.1021/je200628n
Experimental and predicted viscosities of binary mixtures of cyclic ethers with 1-chloropentane or 1-chlorohexane at 293.15, 298.15, and 313.15K:	https://www.doi.org/10.1016/j.tca.2008.11.009
Does Alkyl Chain Length Really Matter? Structure-Property Relationships in Ionic Liquids.:	https://www.doi.org/10.1016/j.tca.2013.04.003
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Densities, Excess Molar Volumes, Viscosities, and Refractive Indices of Binary Mixtures of n-Butyl Acetate with 1-Chloroalkanes (C4 to C8) at 298.15 K:	https://www.doi.org/10.1007/s10765-010-0902-x
Volumetric Study for the Binary Mixtures of Nitromethane with Chloroalkane at Temperatures in the Range (298.15 to 318.15) K:	https://www.doi.org/10.1021/je3013342
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K:	https://www.doi.org/10.1021/je700325c
Speeds of sound, isentropic compressibilities and refractive indices for some binary mixtures of nitromethane with chloroalkane at temperatures from 298.15 to 318.15 K.	https://www.doi.org/10.1016/j.fluid.2014.10.004
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Comparison with theories:	
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1622
Volumetric and optical properties for some (2-butanone + chloroalkane) binary mixtures at T = 298.15 K:	https://www.doi.org/10.1016/j.jct.2014.04.004
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C543599&Units=SI
Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 338.15 K: A comparative study	https://www.doi.org/10.1021/je049652j
Isothermal vapor-liquid equilibria and excess Gibbs free energies in some chloroalkane + chloroalkane mixtures at temperatures from 298.15 K to 318.15 K:	https://www.doi.org/10.1016/j.fluid.2012.10.015
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
connectivity analysis:	

Legend

af:	Acentric Factor
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
kvisc:	Kinematic viscosity
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
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
speedsl:	Speed of sound in fluid
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility