

Hexane, 1,6-dichloro-

Other names:	1,6-Dichlorohexane hexamethylene dichloride
Inchi:	InChI=1S/C6H12Cl2/c7-5-3-1-2-4-6-8/h1-6H2
InchiKey:	OVISMSJCKCDOPU-UHFFFAOYSA-N
Formula:	C6H12Cl2
SMILES:	C1CCCCC1Cl
Mol. weight [g/mol]:	155.06
CAS:	2163-00-0

Physical Properties

Property code	Value	Unit	Source
gf	-24.22	kJ/mol	Joback Method
hf	-198.65	kJ/mol	Joback Method
hfus	19.69	kJ/mol	Joback Method
hvap	37.72	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	3.024		Crippen Method
mvol	119.880	ml/mol	McGowan Method
pc	2865.80	kPa	Joback Method
ripol	1536.00		NIST Webbook
tb	411.54	K	Joback Method
tc	591.61	K	Joback Method
tf	217.22	K	Joback Method
vc	0.469	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.05	J/molxK	471.56	Joback Method
cpg	266.73	J/molxK	591.61	Joback Method
cpg	258.64	J/molxK	561.59	Joback Method
cpg	250.18	J/molxK	531.58	Joback Method
cpg	241.32	J/molxK	501.57	Joback Method
cpg	212.25	J/molxK	411.54	Joback Method

cpg	222.36	J/mol×K	441.55	Joback Method
cpl	243.49	J/mol×K	308.15	Thermodynamic and Acoustic Properties of Mixtures of 1,6-Dichlorohexane with Heptane from (293 to 313) K
cpl	244.00	J/mol×K	310.15	Thermodynamic and Acoustic Properties of Mixtures of 1,6-Dichlorohexane with Heptane from (293 to 313) K
cpl	244.68	J/mol×K	312.15	Thermodynamic and Acoustic Properties of Mixtures of 1,6-Dichlorohexane with Heptane from (293 to 313) K
cpl	244.91	J/mol×K	313.15	Thermodynamic and Acoustic Properties of Mixtures of 1,6-Dichlorohexane with Heptane from (293 to 313) K
cpl	244.35	J/mol×K	311.15	Thermodynamic and Acoustic Properties of Mixtures of 1,6-Dichlorohexane with Heptane from (293 to 313) K
cpl	243.73	J/mol×K	309.15	Thermodynamic and Acoustic Properties of Mixtures of 1,6-Dichlorohexane with Heptane from (293 to 313) K
cpl	237.90	J/mol×K	288.15	Heat Capacities, Densities, and Speeds of Sound for {(1,5-Dichloropentane or 1,6-Dichlorohexane) + Dodecane}

cpl	239.26	J/mol×K	293.15	Heat Capacities, Densities, and Speeds of Sound for {(1,5-Dichloropentane or 1,6-Dichlorohexane) + Dodecane}
cpl	240.60	J/mol×K	298.15	Heat Capacities, Densities, and Speeds of Sound for {(1,5-Dichloropentane or 1,6-Dichlorohexane) + Dodecane}
cpl	241.94	J/mol×K	303.15	Heat Capacities, Densities, and Speeds of Sound for {(1,5-Dichloropentane or 1,6-Dichlorohexane) + Dodecane}
cpl	243.37	J/mol×K	308.15	Heat Capacities, Densities, and Speeds of Sound for {(1,5-Dichloropentane or 1,6-Dichlorohexane) + Dodecane}
cpl	244.81	J/mol×K	313.15	Heat Capacities, Densities, and Speeds of Sound for {(1,5-Dichloropentane or 1,6-Dichlorohexane) + Dodecane}
cpl	246.28	J/mol×K	318.15	Heat Capacities, Densities, and Speeds of Sound for {(1,5-Dichloropentane or 1,6-Dichlorohexane) + Dodecane}
cpl	247.76	J/mol×K	323.15	Heat Capacities, Densities, and Speeds of Sound for {(1,5-Dichloropentane or 1,6-Dichlorohexane) + Dodecane}

cpl	239.21	J/mol×K	293.15	Thermodynamic and Acoustic Properties of Mixtures of 1,6-Dichlorohexane with Heptane from (293 to 313) K
cpl	239.50	J/mol×K	294.15	Thermodynamic and Acoustic Properties of Mixtures of 1,6-Dichlorohexane with Heptane from (293 to 313) K
cpl	239.69	J/mol×K	295.15	Thermodynamic and Acoustic Properties of Mixtures of 1,6-Dichlorohexane with Heptane from (293 to 313) K
cpl	240.02	J/mol×K	296.15	Thermodynamic and Acoustic Properties of Mixtures of 1,6-Dichlorohexane with Heptane from (293 to 313) K
cpl	240.35	J/mol×K	297.15	Thermodynamic and Acoustic Properties of Mixtures of 1,6-Dichlorohexane with Heptane from (293 to 313) K
cpl	240.64	J/mol×K	298.15	Thermodynamic and Acoustic Properties of Mixtures of 1,6-Dichlorohexane with Heptane from (293 to 313) K
cpl	240.85	J/mol×K	299.15	Thermodynamic and Acoustic Properties of Mixtures of 1,6-Dichlorohexane with Heptane from (293 to 313) K

cpl	241.15	J/mol×K	300.15	Thermodynamic and Acoustic Properties of Mixtures of 1,6-Dichlorohexane with Heptane from (293 to 313) K
cpl	241.46	J/mol×K	301.15	Thermodynamic and Acoustic Properties of Mixtures of 1,6-Dichlorohexane with Heptane from (293 to 313) K
cpl	241.80	J/mol×K	302.15	Thermodynamic and Acoustic Properties of Mixtures of 1,6-Dichlorohexane with Heptane from (293 to 313) K
cpl	242.06	J/mol×K	303.15	Thermodynamic and Acoustic Properties of Mixtures of 1,6-Dichlorohexane with Heptane from (293 to 313) K
cpl	242.34	J/mol×K	304.15	Thermodynamic and Acoustic Properties of Mixtures of 1,6-Dichlorohexane with Heptane from (293 to 313) K
cpl	242.62	J/mol×K	305.15	Thermodynamic and Acoustic Properties of Mixtures of 1,6-Dichlorohexane with Heptane from (293 to 313) K
cpl	242.83	J/mol×K	306.15	Thermodynamic and Acoustic Properties of Mixtures of 1,6-Dichlorohexane with Heptane from (293 to 313) K

cpl	243.21	J/molxK	307.15	Thermodynamic and Acoustic Properties of Mixtures of 1,6-Dichlorohexane with Heptane from (293 to 313) K
cpl	236.59	J/molxK	283.15	Heat Capacities, Densities, and Speeds of Sound for {(1,5-Dichloropentane or 1,6-Dichlorohexane) + Dodecane}
dvisc	0.0022422	Paxs	249.61	Joback Method
dvisc	0.0003287	Paxs	411.54	Joback Method
dvisc	0.0004232	Paxs	379.15	Joback Method
dvisc	0.0005713	Paxs	346.77	Joback Method
dvisc	0.0012802	Paxs	281.99	Joback Method
dvisc	0.0046414	Paxs	217.22	Joback Method
dvisc	0.0008204	Paxs	314.38	Joback Method
rfi	1.45550		298.15	Thermodynamic study of (alkyl esters + a,x-alkyl dihalides) I: HE and V E for 25 binary mixtures {xCu-1H2u-1CO2C2H5 + (1-x)a,x-ClCH2(CH2)v-2CH2Cl}, where u = 1 to 5, a = 1 and v = x = 2 to 6
rhof	1063.70	kg/m3	298.15	Excess molar enthalpies and (vapour + liquid) equilibria for mixtures containing N,N-dialkylamides and a,x-dichloroalkanes
rhof	1063.70	kg/m3	298.15	Excess enthalpies and isothermal (vapour + liquid) equilibria of (1-methyl-2-pyrrolidone + 1-chloroalkane or +,?-dichloroalkane) mixtures
srf	0.03	N/m	298.15	The additivity of surface and volumetric properties of alpha,omega-dihalogenoalkanes

srf	0.03	N/m	308.15	The additivity of surface and volumetric properties of alpha,omega-dihalogenoalkanes
srf	0.03	N/m	313.15	The additivity of surface and volumetric properties of alpha,omega-dihalogenoalkanes
srf	0.03	N/m	303.15	The additivity of surface and volumetric properties of alpha,omega-dihalogenoalkanes
srf	0.04	N/m	293.15	The additivity of surface and volumetric properties of alpha,omega-dihalogenoalkanes

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.61007e+01
Coeff. B	-4.63200e+03
Coeff. C	-7.37980e+01
Temperature range (K), min.	366.72
Temperature range (K), max.	503.12

Datasets

Mass density, kg/m³

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m ³ - Liquid
288.15	100.00	1073.7
288.15	500.00	1073.9
288.15	1000.00	1074.3
288.15	1600.00	1074.6

288.15	2000.00	1075.0
288.15	2500.00	1075.3
288.15	3100.00	1075.7
288.15	3600.00	1076.0
288.15	4100.00	1076.3
288.15	4600.00	1076.6
288.15	5100.00	1076.9
288.15	5600.00	1077.3
288.15	6100.00	1077.6
288.15	6500.00	1077.9
288.15	7100.00	1078.3
288.15	7600.00	1078.5
288.15	8100.00	1078.9
288.15	8600.00	1079.2
288.15	9100.00	1079.5
288.15	9600.00	1079.9
288.15	10100.00	1080.2
288.15	10600.00	1080.5
288.15	11100.00	1080.8
288.15	11600.00	1081.2
288.15	12100.00	1081.5
288.15	12600.00	1081.8
288.15	13100.00	1082.1
288.15	13600.00	1082.4
288.15	14200.00	1082.8
288.15	14700.00	1083.0
288.15	15200.00	1083.4
288.15	15700.00	1083.7
288.15	16300.00	1084.0
288.15	16800.00	1084.3
288.15	17300.00	1084.6
288.15	17800.00	1084.9
288.15	18300.00	1085.3
288.15	18800.00	1085.5
288.15	19200.00	1085.7
288.15	19700.00	1086.0
288.15	20200.00	1086.5
298.15	100.00	1063.8
298.15	500.00	1064.2
298.15	1000.00	1064.4
298.15	1500.00	1064.8
298.15	2000.00	1065.2
298.15	2500.00	1065.5
298.15	3100.00	1065.9

298.15	3600.00	1066.3
298.15	4100.00	1066.7
298.15	4500.00	1066.9
298.15	5000.00	1067.3
298.15	5600.00	1067.6
298.15	6100.00	1068.0
298.15	6600.00	1068.4
298.15	7100.00	1068.7
298.15	7600.00	1069.0
298.15	8100.00	1069.4
298.15	8600.00	1069.7
298.15	9200.00	1070.1
298.15	9600.00	1070.4
298.15	10100.00	1070.7
298.15	10600.00	1071.1
298.15	11000.00	1071.3
298.15	11700.00	1071.7
298.15	12100.00	1071.9
298.15	12600.00	1072.3
298.15	13100.00	1072.6
298.15	13600.00	1072.9
298.15	14200.00	1073.3
298.15	14700.00	1073.6
298.15	15200.00	1074.0
298.15	15700.00	1074.3
298.15	16400.00	1074.8
298.15	16800.00	1075.2
298.15	17300.00	1075.5
298.15	17800.00	1075.8
298.15	18300.00	1076.1
298.15	18700.00	1076.4
298.15	19200.00	1076.7
298.15	19700.00	1076.9
298.15	20200.00	1077.3
308.15	100.00	1054.6
308.15	500.00	1054.9
308.15	1000.00	1055.2
308.15	1500.00	1055.5
308.15	2000.00	1055.9
308.15	2500.00	1056.3
308.15	3100.00	1056.7
308.15	3600.00	1057.1
308.15	4100.00	1057.4
308.15	4600.00	1057.8

308.15	5100.00	1058.2
308.15	5600.00	1058.5
308.15	6100.00	1058.9
308.15	6600.00	1059.2
308.15	7100.00	1059.6
308.15	7600.00	1059.8
308.15	8100.00	1060.2
308.15	8600.00	1060.6
308.15	9200.00	1061.0
308.15	9600.00	1061.4
308.15	10100.00	1061.7
308.15	10600.00	1062.1
308.15	11100.00	1062.4
308.15	11600.00	1062.7
308.15	12100.00	1063.1
308.15	12600.00	1063.5
308.15	13100.00	1063.8
308.15	13600.00	1064.1
308.15	14100.00	1064.5
308.15	14800.00	1064.9
308.15	15100.00	1065.1
308.15	15700.00	1065.5
308.15	16200.00	1065.8
308.15	16700.00	1066.2
308.15	17300.00	1066.6
308.15	17800.00	1066.9
308.15	18300.00	1067.2
308.15	18700.00	1067.4
308.15	19200.00	1067.8
308.15	19700.00	1068.0
308.15	20300.00	1068.5
318.15	100.00	1045.1
318.15	500.00	1045.3
318.15	1000.00	1045.7
318.15	1500.00	1046.2
318.15	2000.00	1046.6
318.15	2500.00	1046.9
318.15	3100.00	1047.4
318.15	3600.00	1047.8
318.15	4100.00	1048.1
318.15	4600.00	1048.4
318.15	5100.00	1048.9
318.15	5600.00	1049.2
318.15	6100.00	1049.7

318.15	6600.00	1050.0
318.15	7100.00	1050.4
318.15	7600.00	1050.7
318.15	8100.00	1051.2
318.15	8500.00	1051.4
318.15	9100.00	1051.8
318.15	9600.00	1052.2
318.15	10100.00	1052.6
318.15	10700.00	1053.1
318.15	11100.00	1053.6
318.15	11600.00	1053.9
318.15	12100.00	1054.1
318.15	12600.00	1054.5
318.15	13100.00	1054.8
318.15	13600.00	1055.3
318.15	14200.00	1055.6
318.15	14700.00	1056.0
318.15	15200.00	1056.3
318.15	15600.00	1056.6
318.15	16300.00	1057.1
318.15	16800.00	1057.3
318.15	17300.00	1057.7
318.15	17800.00	1058.0
318.15	18300.00	1058.3
318.15	18900.00	1058.8
318.15	19200.00	1059.0
318.15	19700.00	1059.3
318.15	20200.00	1059.6

Reference

<https://www.doi.org/10.1021/je700339f>

Temperature, K

Pressure, kPa

Mass density, kg/m³

298.15	100.00	1063.8
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Reference

<https://www.doi.org/10.1021/je7003758>

Sources

The additivity of surface and volumetric <https://www.doi.org/10.1016/j.jct.2018.12.042>

properties of <http://webbook.nist.gov/cgi/cbook.cgi?ID=C2163000&Units=SI>
 astatane and dihalogenoalkanes:

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Thermodynamic study of (alkyl esters + a,x-alkyl dihalides) I: HE and V E for 25 The Yaws Handbook of Vapor Pressure: CICH₂(CH₂)_v-2CH₂Cl), where u = 1 to 5 and v = 2 to 6: Properties of Mixtures of 1-Chloroalkane or + 2-Dichloroalkane: Thermodynamic study of (alkyl esters + a,x-alkyl dihalides) VII: HE m and VE m for 25 binary mixtures {x-Cu 1H2u 1CO2C3H7 + (1-x)a,x-CICH₂(CH₂)_v-2CH₂Cl}, where u = 1 to 5 and v = 2 to 6: Heat Capacities, Densities, and Speeds of Sound for (1,5-Dichloroalkane or Chloroalkane) + Dodecane} using the COSMO-RS methodology: Densities and Isothermal Compressibilities at Pressures up to 20 MPa of the systems (alkyl esters + a,x-alkyl dihalides) VIII: HE m and VE m for 25 binary mixtures {x-Cu 1H2u 1CO2C3H7 + (1-x)a,x-CICH₂(CH₂)_v-2CH₂Cl}, where u = 1 to 5 and v = 2 to 6: Densities and Isothermal Compressibilities at Pressures up to 20 MPa of (1,5-Dichloroalkane + 1-Methyl-2-pyrrolidone) + 1-Chloroalkane or + r,u-Dichloroalkane:

<https://www.doi.org/10.1016/j.jct.2005.03.020>
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<https://www.doi.org/10.1021/je100610v>
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<https://www.doi.org/10.1016/j.jct.2005.11.003>
<https://www.doi.org/10.1021/je7003758>

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
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
ripol:	Polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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