

Hexane, 1-bromo-

Other names:	1-Bromohexane 1-Hexyl bromide 1-hexylbromide Bromohexane Hexyl bromide N-HEXYL BROMIDE
Inchi:	InChI=1S/C6H13Br/c1-2-3-4-5-6-7/h2-6H2,1H3
InchiKey:	MNDIARAMWBIKFW-UHFFFAOYSA-N
Formula:	C6H13Br
SMILES:	CCCCCBr
Mol. weight [g/mol]:	165.07
CAS:	111-25-1

Physical Properties

Property code	Value	Unit	Source
chl	-4024.60 ± 1.60	kJ/mol	NIST Webbook
gf	13.96	kJ/mol	Joback Method
hf	-150.10 ± 2.10	kJ/mol	NIST Webbook
hfl	-194.50 ± 1.60	kJ/mol	NIST Webbook
hfus	16.58	kJ/mol	Joback Method
hvap	35.39	kJ/mol	Joback Method
ie	9.91	eV	NIST Webbook
ie	10.06 ± 0.05	eV	NIST Webbook
log10ws	-3.81		Aqueous Solubility Prediction Method
log10ws	-3.81		Estimated Solubility Method
logp	2.962		Crippen Method
mcvol	112.900	ml/mol	McGowan Method
pc	3360.64	kPa	Joback Method
rinpol	935.00		NIST Webbook
rinpol	920.60		NIST Webbook
rinpol	918.30		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	942.00		NIST Webbook
rinpol	960.00		NIST Webbook
rinpol	948.00		NIST Webbook

rinpol	951.00		NIST Webbook
rinpol	964.00		NIST Webbook
rinpol	940.00		NIST Webbook
rinpol	927.00		NIST Webbook
rinpol	938.00		NIST Webbook
rinpol	926.00		NIST Webbook
rinpol	923.00		NIST Webbook
rinpol	923.00		NIST Webbook
rinpol	982.00		NIST Webbook
rinpol	921.40		NIST Webbook
ripol	1167.00		NIST Webbook
ripol	1163.00		NIST Webbook
ripol	1163.00		NIST Webbook
ripol	1156.00		NIST Webbook
ripol	1187.00		NIST Webbook
ripol	1147.00		NIST Webbook
ripol	1159.00		NIST Webbook
ripol	1160.00		NIST Webbook
sl	452.92	J/mol×K	NIST Webbook
tb	429.00 ± 2.00	K	NIST Webbook
tb	430.00 ± 0.25	K	NIST Webbook
tb	428.00	K	NIST Webbook
tb	428.50	K	NIST Webbook
tb	428.50	K	Vapor-liquid equilibrium in the production of the ionic liquid, 1-hexyl-3-methylimidazolium bromide ([HmIm][Br]), in acetone
tb	427.75	K	KDB
tc	586.57	K	Joback Method
tf	188.45 ± 0.60	K	NIST Webbook
tf	188.10 ± 0.20	K	NIST Webbook
tf	188.25	K	Aqueous Solubility Prediction Method
vc	0.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	197.64	J/mol×K	402.84	Joback Method
cpg	208.32	J/mol×K	433.46	Joback Method
cpg	218.53	J/mol×K	464.08	Joback Method

cpg	228.28	J/mol×K	494.70	Joback Method	
cpg	237.59	J/mol×K	525.33	Joback Method	
cpg	246.48	J/mol×K	555.95	Joback Method	
cpg	254.97	J/mol×K	586.57	Joback Method	
cpl	203.55	J/mol×K	298.80	NIST Webbook	
cpl	221.28	J/mol×K	303.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	
cpl	222.90	J/mol×K	308.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	
cpl	224.51	J/mol×K	313.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	
cpl	226.13	J/mol×K	318.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	
cpl	219.66	J/mol×K	298.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	
cpl	229.38	J/mol×K	328.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	
cpl	231.00	J/mol×K	333.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	
cpl	232.62	J/mol×K	338.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	

cpl	234.24	J/mol×K	343.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	235.87	J/mol×K	348.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	237.49	J/mol×K	353.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	239.11	J/mol×K	358.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	240.72	J/mol×K	363.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	242.34	J/mol×K	368.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	243.96	J/mol×K	373.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	245.59	J/mol×K	378.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes

cpl	247.21	J/mol×K	383.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	248.83	J/mol×K	388.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	250.45	J/mol×K	393.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	252.06	J/mol×K	398.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	253.68	J/mol×K	403.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	255.32	J/mol×K	408.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	256.93	J/mol×K	413.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	258.55	J/mol×K	418.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	260.17	J/mol×K	423.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes

cpl	215.54	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
cpl	216.29	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	217.08	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	217.78	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	218.54	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	219.26	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	219.99	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	220.68	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	221.38	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
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cpl	222.22	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
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cpl	222.98	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
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cpl	223.79	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
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cpl	224.63	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	225.37	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	226.20	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	227.01	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	227.86	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
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cpl	228.67	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
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cpl	229.55	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
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cpl	230.39	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
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cpl	231.21	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	231.59	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	233.25	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	233.77	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	234.73	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	235.64	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	236.55	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	237.39	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	237.85	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	219.70	J/mol×K	298.15	NIST Webbook
cpl	227.77	J/mol×K	323.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
dvisc	0.0040640	Pa×s	217.18	Joback Method
dvisc	0.0012430	Pa×s	279.07	Joback Method
dvisc	0.0020875	Pa×s	248.12	Joback Method
dvisc	0.0003465	Pa×s	402.84	Joback Method
dvisc	0.0004403	Pa×s	371.90	Joback Method
dvisc	0.0005844	Pa×s	340.95	Joback Method
dvisc	0.0008208	Pa×s	310.01	Joback Method
hfust	18.05	kJ/mol	188.10	NIST Webbook
hfust	18.05	kJ/mol	188.10	NIST Webbook
hfust	18.05	kJ/mol	188.10	NIST Webbook
hvapt	43.20	kJ/mol	394.50	NIST Webbook
pvap	101.33	kPa	428.50	Vapor-liquid equilibrium in the production of the ionic liquid, 1-hexyl-3-methylimidazolium bromide ([HmIm][Br]), in acetone
rfi	1.44640		298.15	Densities, speeds of sound, isentropic compressibilities, refractive indexes, and viscosities of tetrahydrofuran with haloalkane or alkyl ethanoate at T = 303.15 K

rhoI	1040.90	kg/m3	403.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rhoI	1113.70	kg/m3	343.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rhoI	1137.30	kg/m3	323.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rhoI	1166.80	kg/m3	298.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rhoI	1183.80	kg/m3	283.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rhoI	1195.30	kg/m3	273.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rhoI	1090.80	kg/m3	363.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rhoI	1218.00	kg/m3	253.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rhoI	1066.10	kg/m3	383.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K

sfust	95.98	J/mol×K	188.10	NIST Webbook
sfust	95.98	J/mol×K	188.10	NIST Webbook
speedsl	709.98	m/s	423.23	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	1273.76	m/s	243.60	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	1073.63	m/s	303.20	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	1009.29	m/s	323.20	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	916.03	m/s	353.16	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	826.35	m/s	383.19	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K

speedsl	767.47	m/s	403.25	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	1172.85	m/s	273.31	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.53188e+01
Coeff. B	-3.94571e+03
Coeff. C	-6.02590e+01
Temperature range (K), min.	322.76
Temperature range (K), max.	454.54

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	9.28810e+01
Coeff. B	-8.58497e+03
Coeff. C	-1.14706e+01
Coeff. D	7.01862e-06
Temperature range (K), min.	333.15
Temperature range (K), max.	456.15

Sources

Vapor-liquid equilibrium in the production of the ionic liquid, 1-hexyl-3-methylimidazolium bromide ([HmIm][Br]), in acetone:

<https://www.doi.org/10.1016/j.fluid.2013.11.030>

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
Isobaric heat capacity, isothermal compressibility and fluctuational heat capacities of n-alkanes and 1-bromoalkanes within the temperature range from 298.15 K to 353.15 K. A group additivity and molecular connectivity analysis.	https://www.doi.org/10.1007/s10765-016-2064-y
Densities, speeds of sound, isentropic compressibilities, refractive indexes, and viscosities of n-alkanes with isentropic compressibilities of liquid n-alkanes at temperatures from 240.15 to 420.15 K.	https://www.doi.org/10.1021/je049652j
KDB:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C111251&Units=SI
Estimated Solubility Method:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1633

Legend

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
hfust:	Enthalpy of fusion at a given temperature
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
vpap:	Vapor pressure
rfi:	Refractive Index
rho:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
speedsl:	Speed of sound in fluid

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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