Hexane, 1,6-dibromo-

Other names:	1,6-Dibromo-n-hexane
	1,6-Dibromohexan
	1,6-Dibromohexane
	DBH
	Dibromo-1,6 hexane
	HEXAMETHYLENE DIBROMIDE
Inchi:	InChI=1S/C6H12Br2/c7-5-3-1-2-4-6-8/h1-6H2
InchiKey:	SGRHVVLXEBNBDV-UHFFFAOYSA-N
Formula:	C6H12Br2
SMILES:	BrCCCCCCBr
Mol. weight [g/mol]:	243.97
CAS:	629-03-8

Physical Properties

Property code	Value	Unit	Source
gf	28.28	kJ/mol	Joback Method
hf	-114.51	kJ/mol	Joback Method
hfus	21.87	kJ/mol	Joback Method
hvap	41.82	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	3.337		Crippen Method
mcvol	130.400	ml/mol	McGowan Method
pc	3646.53	kPa	Joback Method
rinpol	1312.00		NIST Webbook
rinpol	1299.00		NIST Webbook
rinpol	1312.00		NIST Webbook
rinpol	1310.00		NIST Webbook
rinpol	1333.00		NIST Webbook
ripol	1807.00		NIST Webbook
ripol	1764.00		NIST Webbook
ripol	1763.00		NIST Webbook
tb	516.00	K	NIST Webbook
tb	516.20	K	NIST Webbook
tc	670.48	K	Joback Method
tf	276.98	K	Joback Method
vc	0.495	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.24	J/mol×K	670.48	Joback Method
cpg	254.18	J/mol×K	536.16	Joback Method
cpg	263.43	J/mol×K	569.74	Joback Method
cpg	272.17	J/mol×K	603.32	Joback Method
cpg	280.43	J/mol×K	636.90	Joback Method
cpg	244.39	J/mol×K	502.58	Joback Method
cpg	234.04	J/mol×K	469.00	Joback Method
cpl	246.41	J/mol×K	294.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	247.20	J/mol×K	297.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	247.47	J/mol×K	298.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	247.60	J/mol×K	298.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K

cpl	248.01	J/mol×K	300.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	248.41	J/mol×K	301.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	248.82	J/mol×K	303.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	249.23	J/mol×K	304.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	249.64	J/mol×K	306.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K

cpl	250.05	J/mol×K	307.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	250.47	J/mol×K	309.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	250.88	J/mol×K	310.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	251.30	J/mol×K	312.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	251.72	J/mol×K	313.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K

cpl	252.15	J/mol×K	315.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	252.57	J/mol×K	316.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	253.00	J/mol×K	318.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	253.42	J/mol×K	319.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	253.85	J/mol×K	321.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K

cpl	254.29	J/mol×K	322.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	254.72	J/mol×K	324.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	255.16	J/mol×K	325.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	255.59	J/mol×K	327.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	256.03	J/mol×K	328.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K

cpl	256.48	J/mol×K	330.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	256.92	J/mol×K	331.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	257.37	J/mol×K	333.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	246.80	J/mol×K	295.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	258.26	J/mol×K	336.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K

cpl	258.71	J/mol×K	337.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	259.17	J/mol×K	339.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	259.62	J/mol×K	340.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	260.08	J/mol×K	342.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	260.54	J/mol×K	343.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K

cpl	261.00	J/mol×K	345.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	261.46	J/mol×K	346.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	261.93	J/mol×K	348.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	262.40	J/mol×K	349.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	262.86	J/mol×K	351.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K

cpl	263.34	J/mol×K	352.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	246.01	J/mol×K	292.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	264.12	J/mol×K	355.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	245.62	J/mol×K	291.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	245.23	J/mol×K	289.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K

cpl	244.84	J/mol×K	288.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	244.45	J/mol×K	286.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	263.81	J/mol×K	354.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	244.06	J/mol×K	285.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	257.81	J/mol×K	334.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
dvisc	0.0004674	Pa×s	437.00	Joback Method
dvisc	0.0031571	Pa×s	276.98	Joback Method
dvisc	0.0018391	Pa×s	308.98	Joback Method
dvisc	0.0011858	Pa×s	340.99	Joback Method
dvisc	0.0003730	Pa×s	469.00	Joback Method
dvisc	0.0006069	Pa×s	404.99	Joback Method

dvisc	0.0008243	Pa×s	372.99	Joback Method
rfi	1.50600		298.15	Thermodynamic study of (alkyl esters + a,x-alkyl dihalides) II: HE m and V E m for 25 binary mixtures {xCu-1H2u-1CO2C2H5 + (1 - x)a,x-BrCH2(CH2)v-2CH2Br}, where u = 1 to 5, a = 1 and v = x = 2 to 6
srf	0.04	N/m	313.15	The additivity of surface and volumetric properties of alpha,omega-dihalogenoalkanes
srf	0.04	N/m	308.15	The additivity of surface and volumetric properties of alpha,omega-dihalogenoalkanes
srf	0.04	N/m	303.15	The additivity of surface and volumetric properties of alpha,omega-dihalogenoalkanes
srf	0.04	N/m	298.15	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(Pvp) = A + B/(T + C)
Coeff. A	1.28647e+01
Coeff. B	-3.64093e+03
Coeff. C	-7.46320e+01
Temperature range (K), min.	364.12
Temperature range (K), max.	556.67

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1632.mol
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Heat Capacity of alpha,omega-Bromochloroalkanes and ?,? Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K:	https://www.doi.org/10.1021/je201002j
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Thermodynamic study of (alkyl esters + alpha,omega-alkyl dihalides) IV: Hex and Vex for 25 binary mixtures {xC(u-1)H(2u-1)CO2CH3 + (1-x)alpha,omega-BrCH2(CH2)v-2CH2Br}, where u = 1 to 5, alpha = 1, and v = omega = 2 to 6:	https://www.doi.org/10.1016/j.jct.2006.05.004
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Thermodynamic study of (alkyl esters + a,x-alkyl dihalides) II: HE m and VE m for 25 binary mixtures {xC(u-1)H(2u-1)CO2C2H5 + (1-x)alpha,omega-BrCH2(CH2)v-2CH2Br}, where u = 1 to 5, alpha = 1, and v = omega = 2 to 6:	https://www.doi.org/10.1016/j.jct.2005.07.009
Thermodynamic study of (alkyl esters + alpha,omega-alkyl dihalides) VI.H and V for 25 binary mixtures {xC(u-1)H(2u-1)CO2(CH2)3CH3 + (1-x)alpha,omega-BrCH2(CH2)v-2CH2Br}, where u = 1 to 5, alpha = 1, and v = omega = 2 to 6:	https://www.doi.org/10.1016/j.jct.2009.05.006
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C629038&Units=SI
The solubility, surface tension, and volumetric properties of alpha,omega-dihalogenoalkanes:	https://www.doi.org/10.1016/j.jct.2018.12.042

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