Heptane, 1-bromo-

Other names:	1-Bromoheptane
	Heptyl bromide
	N-HEPTYL BROMIDE
Inchi:	InChI=1S/C7H15Br/c1-2-3-4-5-6-7-8/h2-7H2,1H3
InchiKey:	LSXKDWGTSHCFPP-UHFFFAOYSA-N
Formula:	C7H15Br
SMILES:	CCCCCCCBr
Mol. weight [g/mol]:	179.10
CAS:	629-04-9

Physical Properties

Property code	Value	Unit	Source
chl	-4679.90 ± 1.60	kJ/mol	NIST Webbook
gf	22.38	kJ/mol	Joback Method
hf	-170.20 ± 2.20	kJ/mol	NIST Webbook
hfl	-218.60 ± 1.60	kJ/mol	NIST Webbook
hfus	19.17	kJ/mol	Joback Method
hvap	50.20	kJ/mol	NIST Webbook
hvap	50.40 ± 0.20	kJ/mol	NIST Webbook
hvap	50.40 ± 0.20	kJ/mol	NIST Webbook
hvap	50.80 ± 0.10	kJ/mol	NIST Webbook
hvap	50.79 ± 0.10	kJ/mol	NIST Webbook
hvap	50.61	kJ/mol	NIST Webbook
ie	9.81	eV	NIST Webbook
log10ws	-4.43		Estimated Solubility Method
log10ws	-4.43		Aqueous Solubility Prediction Method
logp	3.352		Crippen Method
mcvol	126.990	ml/mol	McGowan Method
pc	3015.64	kPa	Joback Method
rinpol	1027.00		NIST Webbook
rinpol	1027.00		NIST Webbook
rinpol	1067.00		NIST Webbook
rinpol	1036.00		NIST Webbook
rinpol	1018.00		NIST Webbook
rinpol	1042.00		NIST Webbook
rinpol	1030.00		NIST Webbook

rinpol	1061.00		NIST Webbook
rinpol	1040.00		NIST Webbook
rinpol	1031.00		NIST Webbook
rinpol	1036.00		NIST Webbook
ripol	1256.00		NIST Webbook
ripol	1256.00		NIST Webbook
ripol	1262.00		NIST Webbook
ripol	1266.00		NIST Webbook
ripol	1282.00		NIST Webbook
ripol	1252.00		NIST Webbook
ripol	1268.00		NIST Webbook
ripol	1262.00		NIST Webbook
tb	451.70	K	NIST Webbook
tb	453.00	K	NIST Webbook
tb	453.20	K	NIST Webbook
tb	453.15	K	KDB
tc	608.13	K	Joback Method
tf	214.90 ± 0.40	K	NIST Webbook
tf	215.82	K	Aqueous Solubility Prediction Method
tf	217.10 ± 0.25	K	NIST Webbook
tf	214.40 ± 0.30	K	NIST Webbook
vc	0.489	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	270.39	J/mol×K	516.93	Joback Method
cpg	300.13	J/mol×K	608.13	Joback Method
cpg	290.67	J/mol×K	577.73	Joback Method
cpg	280.77	J/mol×K	547.33	Joback Method
cpg	259.52	J/mol×K	486.52	Joback Method
cpg	248.15	J/mol×K	456.12	Joback Method
cpg	236.26	J/mol×K	425.72	Joback Method

cpl	253.19	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	264.64	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	262.97	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	262.50	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	265.49	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	261.61	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	260.68	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	259.71	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	258.76	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	257.85	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	255.97	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	255.00	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	266.52	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	267.46	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	268.47	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	254.14	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	269.51	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	270.03	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	247.90	J/mol×K	298.15	NIST Webbook
cpl	249.39	J/mol×K	298.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	251.24	J/mol×K	303.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	253.07	J/mol×K	308.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	254.91	J/mol×K	313.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes

cpl	256.75	J/mol×K	318.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	258.58	J/mol×K	323.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	260.43	J/mol×K	328.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	262.27	J/mol×K	333.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	264.10	J/mol×K	338.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	265.94	J/mol×K	343.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	267.77	J/mol×K	348.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	269.61	J/mol×K	353.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	271.46	J/mol×K	358.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes

cpl	273.29	J/mol×K	363.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	
cpl	275.13	J/mol×K	368.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	
cpl	276.98	J/mol×K	373.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	
cpl	278.80	J/mol×K	378.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	
cpl	280.65	J/mol×K	383.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	
cpl	282.47	J/mol×K	388.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	
cpl	284.32	J/mol×K	393.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	
cpl	286.16	J/mol×K	398.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	

cpl	287.99	J/mol×K	403.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	
cpl	289.83	J/mol×K	408.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	
cpl	291.68	J/mol×K	413.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	
cpl	293.51	J/mol×K	418.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	
cpl	295.35	J/mol×K	423.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	
cpl	244.73	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	245.56	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	246.44	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	247.28	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	248.12	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	248.93	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	249.70	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	250.38	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	251.56	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	252.33	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	256.84	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
dvisc	0.0021013	Pa×s	261.33	Joback Method
dvisc	0.0004213	Pa×s	392.84	Joback Method
dvisc	0.0005640	Pa×s	359.96	Joback Method
dvisc	0.0003293	Pa×s	425.72	Joback Method
dvisc	0.0008006	Pa×s	327.09	Joback Method
dvisc	0.0012290	Pa×s	294.21	Joback Method
dvisc	0.0041928	Pa×s	228.45	Joback Method
hfust	21.76	kJ/mol	214.40	NIST Webbook
hfust	21.76	kJ/mol	214.40	NIST Webbook
hvapt	47.00	kJ/mol	411.00	NIST Webbook
hvapt	47.50	kJ/mol	408.00	NIST Webbook
rhol	1132.90	kg/m3	298.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rhol	1148.70	kg/m3	283.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rhol	1084.50	kg/m3	343.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rhol	1169.60	kg/m3	263.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K

rhol	1191.00	kg/m3	243.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rhol	1106.00	kg/m3	323.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rhol	1159.20	kg/m3	273.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rhol	1026.60	kg/m3	393.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
speedsl	1308.35	m/s	243.74	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	1108.66	m/s	303.19	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	1045.07	m/s	323.14	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K

speedsl	952.86	m/s	353.14	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	863.47	m/s	383.17	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	748.09	m/s	423.22	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	1207.17	m/s	273.33	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(Pvp) = A + B/(T + C)
Coeff. A	1.52868e+01
Coeff. B	-4.12208e+03
Coeff. C	-6.68200e+01
Temperature range (K), min.	341.64
Temperature range (K), max.	480.05

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2

Coeff. A	8.18101e+01
Coeff. B	-8.70223e+03
Coeff. C	-9.62699e+00
Coeff. D	4.55484e-06
Temperature range (K), min.	217.05
Temperature range (K), max.	651.00

Sources

Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K:	https://www.doi.org/10.1021/je700015t
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C629049&Units=SI
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1638.mol
Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 294.15 K to 353.15 K. A group additivity and molecular connectivity analysis:	https://www.doi.org/10.1021/je049652j
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1638
Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K:	https://www.doi.org/10.1021/je900227j
Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1- bromoalkanes:	https://www.doi.org/10.1007/s10765-016-2064-y

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
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
speedsl:	Speed of sound in fluid
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume