

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:	CCCCCCCCBr
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	50.80 ± 0.10	kJ/mol	NIST Webbook
hvap	50.61	kJ/mol	NIST Webbook
hvap	50.40 ± 0.20	kJ/mol	NIST Webbook
hvap	50.79 ± 0.10	kJ/mol	NIST Webbook
hvap	50.40 ± 0.20	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	1061.00		NIST Webbook
rinpol	1027.00		NIST Webbook
rinpol	1027.00		NIST Webbook
rinpol	1030.00		NIST Webbook
rinpol	1040.00		NIST Webbook
rinpol	1031.00		NIST Webbook
rinpol	1067.00		NIST Webbook

rinpol	1036.00		NIST Webbook
rinpol	1018.00		NIST Webbook
rinpol	1042.00		NIST Webbook
rinpol	1036.00		NIST Webbook
ripol	1282.00		NIST Webbook
ripol	1266.00		NIST Webbook
ripol	1262.00		NIST Webbook
ripol	1268.00		NIST Webbook
ripol	1256.00		NIST Webbook
ripol	1256.00		NIST Webbook
ripol	1252.00		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	214.40 ± 0.30	K	NIST Webbook
tf	217.10 ± 0.25	K	NIST Webbook
tf	215.82	K	Aqueous Solubility Prediction Method
tf	214.90 ± 0.40	K	NIST Webbook
vc	0.489	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	236.26	J/molxK	425.72	Joback Method
cpg	248.15	J/molxK	456.12	Joback Method
cpg	259.52	J/molxK	486.52	Joback Method
cpg	270.39	J/molxK	516.93	Joback Method
cpg	280.77	J/molxK	547.33	Joback Method
cpg	290.67	J/molxK	577.73	Joback Method
cpg	300.13	J/molxK	608.13	Joback Method
cpl	247.90	J/molxK	298.15	NIST Webbook
cpl	251.24	J/molxK	303.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes

cpl	253.07	J/molxK	308.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	254.91	J/molxK	313.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	249.39	J/molxK	298.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	258.58	J/molxK	323.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	260.43	J/molxK	328.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	262.27	J/molxK	333.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	264.10	J/molxK	338.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	265.94	J/molxK	343.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	267.77	J/molxK	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/molxK	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/molxK	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/molxK	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/molxK	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/molxK	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	253.19	J/molxK	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	254.14	J/molxK	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	255.00	J/molxK	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	255.97	J/molxK	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	256.84	J/molxK	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	257.85	J/molxK	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	258.76	J/molxK	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	259.71	J/molxK	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	260.68	J/molxK	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	261.61	J/molxK	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	262.50	J/molxK	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	262.97	J/molxK	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	264.64	J/molxK	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	265.49	J/molxK	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	266.52	J/molxK	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/molxK	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/molxK	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	269.51	J/molxK	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/molxK	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	256.75	J/molxK	318.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
dvisc	0.0041928	Paxs	228.45	Joback Method

dvisc	0.0021013	Paxs	261.33	Joback Method
dvisc	0.0012290	Paxs	294.21	Joback Method
dvisc	0.0008006	Paxs	327.09	Joback Method
dvisc	0.0005640	Paxs	359.96	Joback Method
dvisc	0.0004213	Paxs	392.84	Joback Method
dvisc	0.0003293	Paxs	425.72	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
rho1	1084.50	kg/m3	343.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rho1	1169.60	kg/m3	263.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rho1	1191.00	kg/m3	243.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rho1	1026.60	kg/m3	393.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rho1	1132.90	kg/m3	298.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rho1	1106.00	kg/m3	323.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rho1	1159.20	kg/m3	273.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K

rhoI	1148.70	kg/m3	283.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
speedsI	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
speedsI	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
speedsI	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
speedsI	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
speedsI	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
speedsI	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	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
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Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
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	$\ln(P_{vp}) = A + B/T + C*\ln(T) + D*T^2$
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

Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
Density of Gases at Temperatures from (243.15 to 423.15) K
Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes:
NIST Webbook
KDB:
Estimated Solubility Method:

<https://www.doi.org/10.1021/je900227j>
<https://www.doi.org/10.1021/je700015t>
<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>
<https://www.doi.org/10.1007/s10765-016-2064-y>
<http://webbook.nist.gov/cgi/cbook.cgi?ID=C629049&Units=SI>
<https://www.cheric.org/files/research/kdb/mol/mol1638.mol>
http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

The Yaws Handbook of Vapor

Pressure:
Crippen Method:

McGowan Method:

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.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

<http://link.springer.com/article/10.1007/BF02311772>

<https://www.doi.org/10.1021/je049652j>

https://en.wikipedia.org/wiki/Joback_method

<https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1638>

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
rho:	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

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