Octane, 1-bromo-

Other names:	1-Bromooctane
	1-Octylbromide
	N-OCTYL BROMIDE
	Octyl bromide
Inchi:	InChI=1S/C8H17Br/c1-2-3-4-5-6-7-8-9/h2-8H2,1H3
InchiKey:	VMKOFRJSULQZRM-UHFFFAOYSA-N
Formula:	C8H17Br
SMILES:	CCCCCCCCBr
Mol. weight [g/mol]:	193.12
CAS:	111-83-1

Physical Properties

Property code	Value	Unit	Source
chl	-5332.60 ± 2.30	kJ/mol	NIST Webbook
gf	30.80	kJ/mol	Joback Method
hf	-190.10 ± 2.30	kJ/mol	NIST Webbook
hfl	-245.20 ± 2.30	kJ/mol	NIST Webbook
hfus	21.76	kJ/mol	Joback Method
hvap	55.80 ± 0.10	kJ/mol	NIST Webbook
hvap	55.77	kJ/mol	NIST Webbook
hvap	55.10	kJ/mol	NIST Webbook
hvap	55.77 ± 0.25	kJ/mol	NIST Webbook
ie	9.54 ± 0.05	eV	NIST Webbook
ie	9.71	eV	NIST Webbook
log10ws	-5.06		Aqueous Solubility Prediction Method
log10ws	-5.06		Estimated Solubility Method
logp	3.742		Crippen Method
mcvol	141.080	ml/mol	McGowan Method
pc	2721.17	kPa	Joback Method
rinpol	1118.00		NIST Webbook
rinpol	1121.00		NIST Webbook
rinpol	1122.00		NIST Webbook
rinpol	1124.00		NIST Webbook
rinpol	1126.00		NIST Webbook
rinpol	1129.00		NIST Webbook
rinpol	1130.00		NIST Webbook

rinpol	1132.00		NIST Webbook
rinpol	1119.00		NIST Webbook
rinpol	1119.00		NIST Webbook
rinpol	1138.00		NIST Webbook
rinpol	1142.00		NIST Webbook
rinpol	1133.00		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1138.00		NIST Webbook
rinpol	1133.00		NIST Webbook
ripol	1373.00		NIST Webbook
ripol	1385.00		NIST Webbook
ripol	1365.00		NIST Webbook
ripol	1364.00		NIST Webbook
ripol	1351.00		NIST Webbook
ripol	1385.00		NIST Webbook
ripol	1368.00		NIST Webbook
tb	474.65	K	KDB
tb	474.00	K	NIST Webbook
tb	474.00	K	NIST Webbook
tb	471.00 ± 5.00	K	NIST Webbook
tb	474.00 ± 6.00	K	NIST Webbook
tb	474.00	K	NIST Webbook
tc	629.52	K	Joback Method
tf	218.20 ± 0.20	K	NIST Webbook
tf	218.15	K	KDB
vc	0.545	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.10	J/mol×K	448.60	Joback Method
cpg	346.83	J/mol×K	629.52	Joback Method
cpg	336.50	J/mol×K	599.37	Joback Method
cpg	325.68	J/mol×K	569.21	Joback Method
cpg	314.35	J/mol×K	539.06	Joback Method
cpg	302.49	J/mol×K	508.91	Joback Method
cpg	290.08	J/mol×K	478.75	Joback Method

cpl	282.35	J/mol×K	318.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	315.55	J/mol×K	383.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	313.00	J/mol×K	378.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	310.43	J/mol×K	373.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	307.88	J/mol×K	368.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	305.33	J/mol×K	363.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	302.78	J/mol×K	358.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	300.23	J/mol×K	353.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	297.66	J/mol×K	348.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes

cpl	295.11	J/mol×K	343.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	
cpl	292.56	J/mol×K	338.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	
cpl	290.02	J/mol×K	333.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	
cpl	287.47	J/mol×K	328.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	
cpl	284.92	J/mol×K	323.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	
cpl	320.64	J/mol×K	393.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	
cpl	323.19	J/mol×K	398.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	
cpl	325.76	J/mol×K	403.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes	

cpl	328.31	J/mol×K	408.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	330.86	J/mol×K	413.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	333.41	J/mol×K	418.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	335.96	J/mol×K	423.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	272.15	J/mol×K	298.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	274.70	J/mol×K	303.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	277.25	J/mol×K	308.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	279.80	J/mol×K	313.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
cpl	318.10	J/mol×K	388.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes

dvisc	0.0003089	Pa×s	448.60	Joback Method
dvisc	0.0003977	Pa×s	413.79	Joback Method
dvisc	0.0005366	Pa×s	378.97	Joback Method
dvisc	0.0007690	Pa×s	344.16	Joback Method
dvisc	0.0011952	Pa×s	309.35	Joback Method
dvisc	0.0020773	Pa×s	274.53	Joback Method
dvisc	0.0042394	Pa×s	239.72	Joback Method
hfust	24.69	kJ/mol	218.20	NIST Webbook
hfust	24.69	kJ/mol	218.20	NIST Webbook
hvapt	49.30	kJ/mol	424.00	NIST Webbook
rhol	1039.50	kg/m3	363.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rhol	1080.60	kg/m3	323.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rhol	1106.00	kg/m3	298.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rhol	1060.50	kg/m3	343.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rhol	1008.40	kg/m3	393.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rhol	1121.20	kg/m3	283.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K

rhol	1131.20	kg/m3	273.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rhol	1140.90	kg/m3	263.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rhol	1151.10	kg/m3	253.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rhol	1111.00	kg/m3	293.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
speedsl	1336.33	m/s	243.61	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	1235.42	m/s	273.28	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	1137.20	m/s	303.16	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K

speedsl	1073.82	m/s	323.02	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	981.92	m/s	352.91	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	892.87	m/s	382.88	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	835.51	m/s	402.55	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	778.72	m/s	423.04	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	1.54132e+01
Coeff. B	-4.32973e+03
Coeff. C	-7.29080e+01
Temperature range (K), min.	359.16

Temperature range (K), max.	501.52

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.05240e+02
Coeff. B	-1.01903e+04
Coeff. C	-1.30951e+01
Coeff. D	6.94001e-06
Temperature range (K), min.	373.15
Temperature range (K), max.	475.15

Sources

Density of Some 1-Bromoalkanes within the Temperature Range from (248.15 to 429.15) K:	https://www.doi.org/10.1021/je700015t
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
Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes:	https://www.doi.org/10.1007/s10765-016-2064-y
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1643
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1643.mol
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C111831&Units=SI
Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (248.15 to 429.15) K:	https://www.doi.org/10.1021/je900227j
Effect of bromine substitution on the solubility of gases in hydrocarbons and fluorocarbons:	https://www.doi.org/10.1016/j.fluid.2006.11.013

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

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