Propane, 1-bromo-

Other names:	1-Bromopropane
	PROPYL BROMIDE
	UN 2344
	n-C3H7Br
	n-Propyl bromide
Inchi:	InChI=1S/C3H7Br/c1-2-3-4/h2-3H2,1H3
InchiKey:	CYNYIHKIEHGYOZ-UHFFFAOYSA-N
Formula:	C3H7Br
SMILES:	CCCBr
Mol. weight [g/mol]:	122.99
CAS:	106-94-5

Physical Properties

Property code	Value	Unit	Source
af	0.2940		KDB
chl	-2056.60 ± 1.40	kJ/mol	NIST Webbook
gf	-11.30	kJ/mol	Joback Method
hf	-92.00 ± 1.70	kJ/mol	NIST Webbook
hf	-82.93	kJ/mol	NIST Webbook
hfl	-124.40 ± 1.40	kJ/mol	NIST Webbook
hfus	8.81	kJ/mol	Joback Method
hvap	32.13	kJ/mol	NIST Webbook
hvap	31.90 ± 0.10	kJ/mol	NIST Webbook
hvap	31.90 ± 0.08	kJ/mol	NIST Webbook
ie	10.18	eV	NIST Webbook
ie	10.18 ± 0.01	eV	NIST Webbook
ie	10.18 ± 0.01	eV	NIST Webbook
ie	10.18	eV	NIST Webbook
ie	10.20	eV	NIST Webbook
ie	10.21	eV	NIST Webbook
ie	10.49 ± 0.01	eV	NIST Webbook
ie	10.18 ± 0.01	eV	NIST Webbook
log10ws	-1.73		Estimated Solubility Method
log10ws	-1.73		Aqueous Solubility Prediction Method
logp	1.791		Crippen Method

mcvol	70.630	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=2)		KDB
pc	4798.00 ± 20.00	kPa	NIST Webbook
pc	4840.00	kPa	KDB
rinpol	614.00		NIST Webbook
rinpol	640.00		NIST Webbook
rinpol	614.20		NIST Webbook
rinpol	632.00		NIST Webbook
rinpol	618.00		NIST Webbook
rinpol	614.00		NIST Webbook
rinpol	610.00		NIST Webbook
rinpol	636.20		NIST Webbook
rinpol	624.20		NIST Webbook
rinpol	614.00		NIST Webbook
rinpol	632.00		NIST Webbook
rinpol	606.00		NIST Webbook
rinpol	629.00		NIST Webbook
rinpol	601.00		NIST Webbook
rinpol	597.00		NIST Webbook
rinpol	591.00		NIST Webbook
rinpol	649.00		NIST Webbook
rinpol	627.10		NIST Webbook
rinpol	627.70		NIST Webbook
rinpol	635.00		NIST Webbook
rinpol	627.00		NIST Webbook
tb	344.20	K	KDB
tc	536.94 ± 0.10	K	NIST Webbook
tc	544.50	K	NIST Webbook
tc	535.50	K	KDB
tf	163.00 ± 2.00	K	NIST Webbook
tf	163.00	K	KDB
tf	162.70 ± 0.20	K	NIST Webbook
tf	163.15 ± 0.40	K	NIST Webbook
tf	163.20 ± 1.00	K	NIST Webbook
vc	0.266	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	102.51	J/mol×K	365.17	Joback Method

cpg	108.46	J/mol×K	396.14	Joback Method
cpg	114.14	J/mol×K	427.11	Joback Method
cpg	119.55	J/mol×K	458.08	Joback Method
cpg	124.72	J/mol×K	489.05	Joback Method
cpg	129.64	J/mol×K	520.02	Joback Method
cpg	96.29	J/mol×K	334.20	Joback Method
cpl	132.78	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	136.23	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	135.80	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	135.35	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	134.93	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	134.55	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	134.00	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	133.64	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	133.20	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	136.68	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	132.46	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	132.01	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	131.64	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	131.20	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	130.86	J/mol×K	281.65	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	130.48	J/mol×K	279.15	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	130.10	J/mol×K	276.65	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	129.78	J/mol×K	274.15	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	129.02	J/mol×K	269.15	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	137.16	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	137.60	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	138.11	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	138.55	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	134.60	J/mol×K	298.15	NIST Webbook	
cpl	140.20	J/mol×K	298.00	NIST Webbook	
cpl	129.44	J/mol×K	271.65	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	130.50	J/mol×K	298.00	NIST Webbook	
dvisc	0.0031562	Pa×s	183.37	Joback Method	
dvisc	0.0017724	Pa×s	208.51	Joback Method	
dvisc	0.0011268	Pa×s	233.65	Joback Method	

dvisc	0.0007823	Pa×s	258.78	Joback Method
dvisc	0.0005794	Pa×s	283.92	Joback Method
dvisc	0.0004506	Pa×s	309.06	Joback Method
dvisc	0.0003639	Pa×s	334.20	Joback Method
hvapt	29.90	kJ/mol	341.80	NIST Webbook
hvapt	33.60	kJ/mol	344.20	KDB
hvapt	31.80	kJ/mol	322.50	NIST Webbook
hvapt	34.10	kJ/mol	309.00	NIST Webbook
hvapt	31.10 ± 0.10	kJ/mol	322.00	NIST Webbook
hvapt	30.50 ± 0.10	kJ/mol	332.00	NIST Webbook
hvapt	30.10 ± 0.10	kJ/mol	339.00	NIST Webbook
hvapt	29.30 ± 0.10	kJ/mol	352.00	NIST Webbook
hvapt	35.50	kJ/mol	282.00	NIST Webbook
hvapt	32.60	kJ/mol	288.00	NIST Webbook
hvapt	29.84	kJ/mol	344.20	NIST Webbook
rhol	1431.10	kg/m3	243.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rhol	1415.40	kg/m3	253.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rhol	1400.30	kg/m3	263.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rhol	1385.30	kg/m3	273.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K
rhol	1369.40	kg/m3	283.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K

rhol	1344.50	kg/m3	298.15	Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K	
speedsl	1075.02	m/s	263.38	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K	
speedsl	1040.10	m/s	273.31	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K	
speedsl	1144.84	m/s	243.76	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K	
speedsl	1005.51	m/s	283.26	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K	
speedsl	971.22	m/s	293.22	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K	
speedsl	954.05	m/s	298.21	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K	

speedsl	870.16	m/s	323.21	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	804.19	m/s	343.21	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	739.38	m/s	363.23	Speed of Sound, Densities, and Isentropic Compressibilities of Liquid 1-Bromoalkanes at Temperatures from (243.15 to 423.15) K
speedsl	674.94	m/s	383.47	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	1.48914e+01
Coeff. B	-3.23755e+03
Coeff. C	-2.87500e+01
Temperature range (K), min.	250.44
Temperature range (K), max.	367.04

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

Coeff. A	7.52251e+01
Coeff. B	-6.17233e+03
Coeff. C	-9.19579e+00
Coeff. D	8.71010e-06
Temperature range (K), min.	163.15
Temperature range (K), max.	544.00

Sources

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
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB Pure (Korean Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1592
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1592.mol
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1592
Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K:	https://www.doi.org/10.1021/je700015t
Solubilities of Lauric Acid in n-Hexane, Acetone, Propanol, 2-Propanol, 1-Bromopropane, and Trichloroethylene from (279.0 to 315.3) K:	https://www.doi.org/10.1021/je800739y
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C106945&Units=SI
Solubilities of Fatty Acids and Triglycerides in 1-Bromopropane:	https://www.doi.org/10.1021/je201181k

Legend

af:	Acentric Factor
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
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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-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