Methane, bromotrichloro-

Other names:	Bromotrichloromethane
	CARBON BROMOTRICHLORIDE
	CCl3Br
	Carbon trichlorobromide
	Monobromotrichloromethane
	TRICHLOROMETHYL BROMIDE
	Trichlorobromomethane
Inchi:	InChI=1S/CBrCl3/c2-1(3,4)5
InchiKey:	XNNQFQFUQLJSQT-UHFFFAOYSA-N
Formula:	CBrCl3
SMILES:	ClC(Cl)(Cl)Br
Mol. weight [g/mol]:	198.27
CAS:	75-62-7

Physical Properties

Property code	Value	Unit	Source
gf	-61.09	kJ/mol	Joback Method
hf	-42.00 ± 1.00	kJ/mol	NIST Webbook
hf	-39.00	kJ/mol	NIST Webbook
hfus	8.81	kJ/mol	Joback Method
hvap	36.11	kJ/mol	Joback Method
ie	10.91	eV	NIST Webbook
ie	11.05 ± 0.02	eV	NIST Webbook
ie	10.60	eV	NIST Webbook
log10ws	-2.73		Crippen Method
logp	2.709		Crippen Method
mcvol	79.170	ml/mol	McGowan Method
pc	5594.19	kPa	Joback Method
rinpol	750.00		NIST Webbook
rinpol	757.00		NIST Webbook
rinpol	754.00		NIST Webbook
rinpol	762.00		NIST Webbook
rinpol	772.00		NIST Webbook
ripol	1087.48		NIST Webbook
ripol	1070.00		NIST Webbook
ripol	1070.00		NIST Webbook
ripol	1075.59		NIST Webbook

ripol	1101.23		NIST Webbook
tb	376.65 ± 2.00	K	NIST Webbook
tc	629.91	K	Joback Method
tf	268.00 ± 0.02	K	NIST Webbook
vc	0.289	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	92.41	J/mol×K	397.50	Joback Method
cpg	95.26	J/mol×K	436.23	Joback Method
cpg	97.63	J/mol×K	474.97	Joback Method
cpg	99.57	J/mol×K	513.70	Joback Method
cpg	101.12	J/mol×K	552.44	Joback Method
cpg	102.34	J/mol×K	591.17	Joback Method
cpg	103.25	J/mol×K	629.91	Joback Method
cpl	149.40	J/mol×K	298.00	NIST Webbook
dvisc	0.0005797	Pa×s	397.50	Joback Method
dvisc	0.0028102	Pa×s	277.09	Joback Method
dvisc	0.0046146	Pa×s	253.01	Joback Method
dvisc	0.0012990	Pa×s	325.25	Joback Method
dvisc	0.0009566	Pa×s	349.34	Joback Method
dvisc	0.0007328	Pa×s	373.42	Joback Method
dvisc	0.0018526	Pa×s	301.17	Joback Method
hfust	2.54	kJ/mol	267.50	NIST Webbook
hfust	4.62	kJ/mol	238.20	NIST Webbook
hfust	0.53	kJ/mol	259.30	NIST Webbook
hfust	2.03	kJ/mol	267.90	NIST Webbook
hvapt	35.00	kJ/mol	330.00	NIST Webbook
hvapt	36.10	kJ/mol	368.50	NIST Webbook

rhol	2002.14	kg/m3	298.15	Vapour liquid equilibrium at T = 308.15 K for binary systems: Dibromomethane + n-heptane, bromotrichloromethane + n-heptane, bromotrichloromethane + dibromomethane, bromotrichloromethane + bromochloromethane and dibromomethane + bromochloromethane. Experimental data and modelling
sfust	19.40	J/mol×K	238.20	NIST Webbook
sfust	2.03	J/mol×K	259.30	NIST Webbook
sfust	7.58	J/mol×K	267.90	NIST Webbook
speedsl	903.60	m/s	298.15	Excess Molar Volumes and Speed of Sound in Bromotrichloromethane + n-Heptane, Dibromomethane + n-Heptane, Bromotrichloromethane + Dibromomethane, and Bromotrichloromethane + Bromochloromethane at Temperatures from (293.15 to 313.15) K
speedsl	917.10	m/s	293.15	Excess Molar Volumes and Speed of Sound in Bromotrichloromethane + n-Heptane, Dibromomethane + n-Heptane, Bromotrichloromethane + Dibromomethane, and Bromotrichloromethane + Bromochloromethane at Temperatures from (293.15 to 313.15) K

speedsl	917.10	m/s	293.15	Excess Molar Volumes and Speed of Sound in Bromotrichloromethane + n-Heptane, Dibromomethane + n-Heptane, Bromotrichloromethane + Dibromomethane, and Bromotrichloromethane + Bromochloromethane at Temperatures from (293.15 to 313.15) K
speedsl	903.60	m/s	298.15	Excess Molar Volumes and Speed of Sound in Bromotrichloromethane + n-Heptane, Dibromomethane + n-Heptane, Bromotrichloromethane + Dibromomethane, and Bromotrichloromethane + Bromochloromethane at Temperatures from (293.15 to 313.15) K
speedsl	903.60	m/s	298.15	Excess Molar Volumes and Speed of Sound in Bromotrichloromethane + n-Heptane, Dibromomethane + n-Heptane, Bromotrichloromethane + Dibromomethane, and Bromotrichloromethane + Bromochloromethane at Temperatures from (293.15 to 313.15) K

speedsl	917.10	m/s	293.15	Excess Molar Volumes and Speed of Sound in Bromotrichloromethane + n-Heptane, Dibromomethane + n-Heptane, Bromotrichloromethane + Dibromomethane, and Bromotrichloromethane + Bromochloromethane at Temperatures from (293.15 to 313.15) K
speedsl	890.20	m/s	303.15	Excess Molar Volumes and Speed of Sound in Bromotrichloromethane + n-Heptane, Dibromomethane + n-Heptane, Bromotrichloromethane + Dibromomethane, and Bromotrichloromethane + Bromochloromethane at Temperatures from (293.15 to 313.15) K
speedsl	890.20	m/s	303.15	Excess Molar Volumes and Speed of Sound in Bromotrichloromethane + n-Heptane, Dibromomethane + n-Heptane, Bromotrichloromethane + Dibromomethane, and Bromotrichloromethane + Bromochloromethane at Temperatures from (293.15 to 313.15) K

speedsl	890.20	m/s	303.15	Excess Molar Volumes and Speed of Sound in Bromotrichloromethane + n-Heptane, Dibromomethane + n-Heptane, Bromotrichloromethane + Dibromomethane, and Bromotrichloromethane + Bromochloromethane at Temperatures from (293.15 to 313.15) K
speedsl	876.80	m/s	308.15	Excess Molar Volumes and Speed of Sound in Bromotrichloromethane + n-Heptane, Dibromomethane + n-Heptane, Bromotrichloromethane + Dibromomethane, and Bromotrichloromethane + Bromochloromethane at Temperatures from (293.15 to 313.15) K
speedsl	876.80	m/s	308.15	Excess Molar Volumes and Speed of Sound in Bromotrichloromethane + n-Heptane, Dibromomethane + n-Heptane, Bromotrichloromethane + Dibromomethane, and Bromotrichloromethane + Bromochloromethane at Temperatures from (293.15 to 313.15) K

speedsl	876.80	m/s	308.15	Excess Molar Volumes and Speed of Sound in Bromotrichloromethane + n-Heptane, Dibromomethane + n-Heptane, Bromotrichloromethane + Dibromomethane, and Bromotrichloromethane + Bromochloromethane at Temperatures from (293.15 to 313.15) K
speedsl	863.60	m/s	313.15	Excess Molar Volumes and Speed of Sound in Bromotrichloromethane + n-Heptane, Dibromomethane + n-Heptane, Bromotrichloromethane + Dibromomethane, and Bromotrichloromethane + Bromochloromethane at Temperatures from (293.15 to 313.15) K
speedsl	863.60	m/s	313.15	Excess Molar Volumes and Speed of Sound in Bromotrichloromethane + n-Heptane, Dibromomethane + n-Heptane, Bromotrichloromethane + Dibromomethane, and Bromotrichloromethane + Bromochloromethane at Temperatures from (293.15 to 313.15) K

speedsl	863.60	m/s	313.15	Excess Molar Volumes and Speed of Sound in Bromotrichloromethane + n-Heptane, Dibromomethane + n-Heptane, Bromotrichloromethane + Dibromomethane, and Bromotrichloromethane + Bromochloromethane at Temperatures from (293.15 to 313.15) K

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45069e+01
Coeff. B	-3.38195e+03
Coeff. C	-3.46430e+01
Temperature range (K), min.	252.15
Temperature range (K), max.	404.31

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	5.19744e+01
Coeff. B	-5.77070e+03
Coeff. C	-5.48617e+00
Coeff. D	3.26165e-06
Temperature range (K), min.	252.15
Temperature range (K), max.	606.00

Sources

KDB: https://www.cheric.org/files/research/kdb/mol/mol1501.mol

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Vapour liquid equilibrium at T = 308.15 K for binary systems: Dibromomethane + n-heptane, bromotrichloromethane + n-heptane, bromotrichloromethane + dibromomethane,	https://www.doi.org/10.1016/j.fluid.2015.03.023
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75627&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Excess Molar Volumes and Speed of Sound in Bromotrichloromethane + n-Heptane, Dibromomethane + n-Heptane, Bromotrichloromethane + Dibromomethane and Bromochloromethane + Dibromomethane at Temperatures from (293.15 to 313.15) K:	https://www.doi.org/10.1021/je300775u
bromotrichloromethane + bromochloromethane and dibromomethane + bromochloromethane, Experimental data and modelling:	https://en.wikipedia.org/wiki/Joback_method
Relation between characteristic molecular volume and hydrophobicity of halogenated methanes:	https://www.doi.org/10.1016/j.jct.2010.04.011
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1501
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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
sfust:	Entropy of fusion at a given temperature
speedsl:	Speed of sound in fluid
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume