Methane, bromochloro-

Other names:	Bromochloromethane
	CBM
	CH2ClBr
	Chlorobromomethane
	Fluorocarbon 1011
	HALON 1011
	MIL-B-4394-B
	Methylene bromide chloride
	Methylene chlorobromide
	Monochloromonobromomethane
	NSC 7294
	REFRIGERANT-30B1
	UN 1887
Inchi:	InChI=1S/CH2BrCl/c2-1-3/h1H2
InchiKey:	JPOXNPPZZKNXOV-UHFFFAOYSA-N
Formula:	CH2BrCl
SMILES:	ClCBr
Mol. weight [g/mol]:	129.38
CAS:	74-97-5

Physical Properties

Property code	Value	Unit	Source
gf	-40.07	kJ/mol	Joback Method
hf	-20.00 ± 7.00	kJ/mol	NIST Webbook
hfus	7.83	kJ/mol	Joback Method
hvap	28.64	kJ/mol	Joback Method
ie	10.75 ± 0.05	eV	NIST Webbook
ie	10.77 ± 0.01	eV	NIST Webbook
ie	10.77	eV	NIST Webbook
ie	10.77 ± 0.01	eV	NIST Webbook
log10ws	-0.89		Estimated Solubility Method
log10ws	-0.89		Aqueous Solubility Prediction Method
logp	1.578		Crippen Method
mcvol	54.690	ml/mol	McGowan Method
pc	6084.49	kPa	Joback Method

rinpol	575.00		NIST Webbook
rinpol	598.00		NIST Webbook
rinpol	578.00		NIST Webbook
rinpol	598.00		NIST Webbook
rinpol	617.00		NIST Webbook
rinpol	578.00		NIST Webbook
rinpol	569.00		NIST Webbook
rinpol	607.00		NIST Webbook
rinpol	611.00		NIST Webbook
rinpol	607.00		NIST Webbook
rinpol	582.00		NIST Webbook
rinpol	598.00		NIST Webbook
rinpol	602.00		NIST Webbook
ripol	1064.58		NIST Webbook
ripol	1066.29		NIST Webbook
ripol	1057.80		NIST Webbook
ripol	1054.00		NIST Webbook
ripol	1060.00		NIST Webbook
ripol	1054.00		NIST Webbook
tb	341.00	K	NIST Webbook
tb	342.00	K	NIST Webbook
tc	522.75	K	Joback Method
tf	185.20 ± 0.05	K	NIST Webbook
tf	185.18	K	Aqueous Solubility Prediction Method
vc	0.203	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	65.39	J/mol×K	424.31	Joback Method
cpg	60.91	J/mol×K	358.68	Joback Method
cpg	58.44	J/mol×K	325.87	Joback Method
cpg	67.40	J/mol×K	457.12	Joback Method
cpg	69.28	J/mol×K	489.93	Joback Method
cpg	71.04	J/mol×K	522.75	Joback Method
cpg	63.23	J/mol×K	391.50	Joback Method
dvisc	0.0017389	Pa×s	213.27	Joback Method
dvisc	0.0011827	Pa×s	235.79	Joback Method
dvisc	0.0008603	Pa×s	258.31	Joback Method
dvisc	0.0006586	Pa×s	280.83	Joback Method

dvisc	0.0005246	Pa×s	303.35	Joback Method
dvisc	0.0028003	Pa×s	190.75	Joback Method
dvisc	0.0004312	Pa×s	325.87	Joback Method
hvapt	33.50	kJ/mol	315.00	NIST Webbook
hvapt	42.00	kJ/mol	283.50	NIST Webbook
pvap	37.28	kPa	313.15	Isothermal Vapor-Liquid Equilibria of ethyl acetate + dibromomethane, or + bromochloromethane or + 1,2-dichloroethane or +1-bromo-2-chloroethane at T = 313.15 K
rhol	1921.71	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
rhol	1924.55	kg/m3	298.15	(Vapor + liquid) equilibria for the binary mixtures (1-propanol + dibromomethane, or + bromochloromethane, or + 1,2-dichloroethane or +1-bromo-2-chloroethane) at T = 313.15 K.

speedsl	1001.20	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	940.80	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	955.90	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	971.00	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	986.10	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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48065e+01
Coeff. B	-3.12475e+03
Coeff. C	-3.44960e+01
Temperature range (K), min.	249.72
Temperature range (K), max.	363.59

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.51479e+01

Coeff. B	-5.95434e+03
Coeff. C	-7.49956e+00
Coeff. D	5.73549e-06
Temperature range (K), min.	185.20
Temperature range (K), max.	557.00

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C74975&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
(Vapor + liquid) equilibria for the binary mixtures (1-propanol + dibromomethane, or + bromochloromethane, or + 1,2-dichloroethane or 1-bromo-2-chloroethane) at T = 313.15 K.:	https://www.doi.org/10.1016/j.jct.2004.07.012
Temperature and Pressure Dependence of the Volumetric Properties of Binary Liquid Mixtures Containing Dihaloalkanes:	https://www.doi.org/10.1007/s10765-005-5570-x
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Excess Molar Volumes and Speed of Sound in Bromotrichloromethane + n-Heptane, Dibromomethane + n-Heptane, Bromotrichloromethane + Dibromomethane, and Bromochloromethane + Bromotrichloromethane at Temperatures ...:	https://www.doi.org/10.1021/je300775u
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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1523.mol
Isothermal Vapor-Liquid Equilibria of ...:	https://www.doi.org/10.1021/je034259j
Determination of Henry's Law Constants Using Internal Standards with Benchmark Values:	https://www.doi.org/10.1021/je3010535
... ethyl acetate + dibromomethane, or + bromochloromethane, or + 1,2-dichloroethane or ... at T = 313.15 K.:	http://link.springer.com/article/10.1007/BF02311772
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1523

Legend

cpg:	Ideal gas 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
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