Methane, tribromo-

Other names:	BROMOFORM
	Bromoforme
	Bromoformio
	CHBr3
	Methenyl tribromide
	NCI-C55130
	NSC 8019
	REFRIGERANT-20B3
	Rcra waste number U225
	TRIBROMOMETHANE
	Tribrommethaan
	Tribrommethan
	Tribromometan
	UN 2515
Inchi:	InChI=1S/CHBr3/c2-1(3)4/h1H
InchiKey:	DIKBFYAXUHHXCS-UHFFFAOYSA-N
Formula:	CHBr3
SMILES:	BrC(Br)Br
Mol. weight [g/mol]:	252.73
CAS:	75-25-2

Physical Properties

Property code	Value	Unit	Source
chl	-545.80 ± 3.30	kJ/mol	NIST Webbook
gf	-1.94	kJ/mol	Joback Method
hf	55.40 ± 3.30	kJ/mol	NIST Webbook
hfl	9.40 ± 3.30	kJ/mol	NIST Webbook
hfus	10.68	kJ/mol	Joback Method
hvap	46.06	kJ/mol	NIST Webbook
hvap	46.05 ± 0.10	kJ/mol	NIST Webbook
hvap	46.10 ± 0.10	kJ/mol	NIST Webbook
ie	10.47	eV	NIST Webbook
ie	10.47	eV	NIST Webbook
ie	10.47	eV	NIST Webbook
ie	10.51 ± 0.02	eV	NIST Webbook
ie	10.48 ± 0.02	eV	NIST Webbook
ie	10.70 ± 0.30	eV	NIST Webbook

ie	10.50 ± 0.02	eV	NIST Webbook
ie	10.50	eV	NIST Webbook
log10ws	-1.91		Estimated Solubility Method
log10ws	-1.91		Aqueous Solubility Prediction Method
logp	2.455		Crippen Method
mcvol	77.450	ml/mol	McGowan Method
pc	8279.51	kPa	Joback Method
rinpol	852.00		NIST Webbook
rinpol	860.00		NIST Webbook
rinpol	853.00		NIST Webbook
rinpol	852.00		NIST Webbook
rinpol	911.00		NIST Webbook
rinpol	875.00		NIST Webbook
rinpol	875.00		NIST Webbook
rinpol	877.00		NIST Webbook
rinpol	853.00		NIST Webbook
rinpol	852.70		NIST Webbook
rinpol	892.10		NIST Webbook
rinpol	845.20		NIST Webbook
rinpol	873.10		NIST Webbook
rinpol	895.00		NIST Webbook
rinpol	859.00		NIST Webbook
rinpol	882.00		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	852.00		NIST Webbook
rinpol	855.00		NIST Webbook
rinpol	892.00		NIST Webbook
ripol	1456.67		NIST Webbook
ripol	1407.00		NIST Webbook
ripol	1407.00		NIST Webbook
ripol	1418.00		NIST Webbook
ripol	1441.60		NIST Webbook
ripol	1467.06		NIST Webbook
ripol	1456.67		NIST Webbook
tb	422.33	K	KDB
tc	661.75	K	Joback Method
tf	281.20	K	KDB
tf	281.65	K	Aqueous Solubility Prediction Method
tt	281.84 ± 0.02	K	NIST Webbook
vc	0.272	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	80.84	J/mol×K	420.32	Joback Method
cpg	91.09	J/mol×K	661.75	Joback Method
cpg	89.98	J/mol×K	621.52	Joback Method
cpg	88.68	J/mol×K	581.28	Joback Method
cpg	87.16	J/mol×K	541.04	Joback Method
cpg	85.37	J/mol×K	500.80	Joback Method
cpg	83.28	J/mol×K	460.56	Joback Method
cpl	135.10	J/mol×K	298.00	NIST Webbook
cpl	130.50	J/mol×K	298.00	NIST Webbook
dvisc	0.0021459	Pa×s	291.25	Joback Method
dvisc	0.0014934	Pa×s	317.06	Joback Method
dvisc	0.0010976	Pa×s	342.88	Joback Method
dvisc	0.0008422	Pa×s	368.69	Joback Method
dvisc	0.0006691	Pa×s	394.50	Joback Method
dvisc	0.0033088	Pa×s	265.43	Joback Method
dvisc	0.0005468	Pa×s	420.32	Joback Method
hfust	11.05	kJ/mol	281.84	NIST Webbook
hfust	11.09	kJ/mol	281.50	NIST Webbook
hfust	11.10	kJ/mol	281.50	NIST Webbook
hvapt	44.00	kJ/mol	338.00	NIST Webbook
hvapt	42.30	kJ/mol	366.00	NIST Webbook
hvapt	39.66	kJ/mol	422.30	NIST Webbook
sfust	39.20	J/mol×K	281.84	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41922e+01
Coeff. B	-3.48160e+03
Coeff. C	-5.83450e+01
Temperature range (K), min.	281.20
Temperature range (K), max.	450.86

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.41982e+01
Coeff. B	-7.67473e+03
Coeff. C	-8.62341e+00
Coeff. D	4.08397e-06
Temperature range (K), min.	281.20
Temperature range (K), max.	696.00

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1514
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1514
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Determination of Henry's Law Constants Using Internal Standards With Benchmark Values:	https://www.doi.org/10.1021/je3010535
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75252&Units=SI
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Solubility of Halogenated Hydrocarbons in Hydrophobic Ionic Liquids: Experimental Study and COSMO-RS Prediction:	https://www.doi.org/10.1021/acs.jced.5b00310
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume