Chloromethane

Other names:	Artic
	CH3Cl
	Chloor-methaan
	Chlor-methan
	Chlorure de methyle
	Clorometano
	Cloruro di metile
	Freon 40
	Methane, chloro-
	Methyl chloride
	Methylchlorid
	Metylu chlorek
	Monochloromethane
	R 40
	R-40
	Rcra waste number U045
	Refrigerant R40
	UN 1063
Inchi:	InChI=1S/CH3Cl/c1-2/h1H3
InchiKey:	NEHMKBQYUWJMIP-UHFFFAOYSA-N
Formula:	CH3Cl
SMILES:	CCl
Mol. weight [g/mol]:	50.49
CAS:	74-87-3

Physical Properties

Property code	Value	Unit	Source
affp	647.30	kJ/mol	NIST Webbook
basg	621.10	kJ/mol	NIST Webbook
chg	-764.00 ± 0.50	kJ/mol	NIST Webbook
gf	-54.39	kJ/mol	Joback Method
hf	-85.90 ± 0.59	kJ/mol	NIST Webbook
hf	-81.90 ± 1.50	kJ/mol	NIST Webbook
hf	-81.96 ± 0.67	kJ/mol	NIST Webbook
hfl	-102.40 ± 1.50	kJ/mol	NIST Webbook
hfus	2.54	kJ/mol	Joback Method
hvap	20.50 ± 0.30	kJ/mol	NIST Webbook

ie	11.33	eV	NIST Webbook
ie	11.27	eV	NIST Webbook
ie	11.22 ± 0.01	eV	NIST Webbook
ie	11.30	eV	NIST Webbook
ie	11.28 ± 0.01	eV	NIST Webbook
ie	11.28	eV	NIST Webbook
ie	11.29	eV	NIST Webbook
ie	11.29	eV	NIST Webbook
ie	11.22	eV	NIST Webbook
ie	11.28 ± 0.01	eV	NIST Webbook
ie	11.27 ± 0.00	eV	NIST Webbook
ie	11.29	eV	NIST Webbook
ie	11.26	eV	NIST Webbook
ie	11.26 ± 0.03	eV	NIST Webbook
log10ws	-0.88		Aqueous Solubility Prediction Method
logp	0.855		Crippen Method
mcvol	37.190	ml/mol	McGowan Method
pc	6680.00 ± 202.65	kPa	NIST Webbook
pc	6679.24 ± 4.05	kPa	NIST Webbook
pc	6714.40 ± 0.67	kPa	NIST Webbook
pc	7400.00 ± 303.98	kPa	NIST Webbook
pt	0.87 ± 0.00	kPa	NIST Webbook
rhoc	362.98 ± 0.30	kg/m3	NIST Webbook
rhoc	370.08 ± 5.05	kg/m3	NIST Webbook
rinpol	340.00		NIST Webbook
rinpol	332.00		NIST Webbook
rinpol	332.00		NIST Webbook
rinpol	332.00		NIST Webbook
rinpol	332.92		NIST Webbook
rinpol	332.92		NIST Webbook
rinpol	329.00		NIST Webbook
rinpol	327.00		NIST Webbook
rinpol	332.00		NIST Webbook
rinpol	326.00		NIST Webbook
rinpol	326.00		NIST Webbook
rinpol	332.00		NIST Webbook
rinpol	324.00		NIST Webbook
rinpol	329.00		NIST Webbook
sl	140.08	J/mol×K	NIST Webbook
tb	259.71	K	Joback Method
tc	427.76	K	Joback Method
tf	175.80	K	Aqueous Solubility Prediction Method
tf	176.50 ± 0.50	K	NIST Webbook

tf	175.55 ± 0.40	K	NIST Webbook
tf	182.00 ± 1.50	K	NIST Webbook
tt	175.44 ± 0.05	K	NIST Webbook
tt	175.43 ± 0.07	K	NIST Webbook
vc	0.141	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	49.56	J/mol×K	399.76	Joback Method
cpg	39.03	J/mol×K	259.71	Joback Method
cpg	41.27	J/mol×K	287.72	Joback Method
cpg	43.44	J/mol×K	315.73	Joback Method
cpg	45.54	J/mol×K	343.74	Joback Method
cpg	47.58	J/mol×K	371.75	Joback Method
cpg	51.48	J/mol×K	427.76	Joback Method
cpl	81.20	J/mol×K	298.00	NIST Webbook
cpl	75.60	J/mol×K	249.67	NIST Webbook
cpl	80.80	J/mol×K	293.15	NIST Webbook
dvisc	0.0003840	Pa×s	195.33	Joback Method
dvisc	0.0005526	Pa×s	173.87	Joback Method
dvisc	0.0008810	Pa×s	152.41	Joback Method
dvisc	0.0001849	Pa×s	259.71	Joback Method
dvisc	0.0002258	Pa×s	238.25	Joback Method
dvisc	0.0002868	Pa×s	216.79	Joback Method
dvisc	0.0016364	Pa×s	130.95	Joback Method
hfust	6.43	kJ/mol	175.44	NIST Webbook
hfust	6.43	kJ/mol	174.50	NIST Webbook
hfust	6.42	kJ/mol	174.50	NIST Webbook
hsubt	31.60 ± 0.10	kJ/mol	151.00	NIST Webbook
hvapt	22.00	kJ/mol	238.00	NIST Webbook
hvapt	23.50	kJ/mol	220.00	NIST Webbook
hvapt	22.60	kJ/mol	220.50	NIST Webbook
hvapt	20.09	kJ/mol	293.00	NIST Webbook
hvapt	21.54	kJ/mol	248.94	NIST Webbook
hvapt	20.10	kJ/mol	293.00	NIST Webbook
hvapt	22.70	kJ/mol	216.50	NIST Webbook
hvapt	21.00	kJ/mol	340.50	NIST Webbook
hvapt	21.80	kJ/mol	392.00	NIST Webbook
hvapt	22.00	kJ/mol	278.50	NIST Webbook

pvap	260.10	kPa	273.10	Vapor-Liquid Equilibria on Seven Binary Systems: Ethylene Oxide + 2-Methylpropane; Acetophenone + Phenol; cis-1,3-Dichloropropene + 1,2-Dichloropropane; 1,5-Hexadiene + Allyl Chloride; Isopropyl Acetate + Acetonitrile; Vinyl Chloride + Methyl Chloride; and 1,4-Butanediol + c-Butyrolactone
pvap	870.90	kPa	313.15	Vapor-Liquid Equilibria on Seven Binary Systems: Ethylene Oxide + 2-Methylpropane; Acetophenone + Phenol; cis-1,3-Dichloropropene + 1,2-Dichloropropane; 1,5-Hexadiene + Allyl Chloride; Isopropyl Acetate + Acetonitrile; Vinyl Chloride + Methyl Chloride; and 1,4-Butanediol + c-Butyrolactone
sfust	36.66	J/mol×K	175.44	NIST Webbook
svapt	86.51	J/mol×K	248.94	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43821e+01
Coeff. B	-2.04489e+03
Coeff. C	-3.75640e+01
Temperature range (K), min.	175.45
Temperature range (K), max.	376.25

Datasets

Specific volume, m3/kg

Temperature, K - Liquid	Pressure, kPa - Liquid	Specific volume, m3/kg - Liquid
298.00	10000.00	0.0011
298.00	20000.00	0.0010
298.00	30000.00	0.0010
298.00	40000.00	0.0010
298.00	50000.00	0.0010
298.00	75000.00	0.0010
298.00	100000.00	0.0010
298.00	125000.00	0.0009
298.00	150000.00	0.0009
298.00	175000.00	0.0009
298.00	200000.00	0.0009
298.00	225000.00	0.0009
298.00	250000.00	0.0009
298.00	275000.00	0.0009
298.00	300000.00	0.0009
298.00	325000.00	0.0009
298.00	350000.00	0.0008
298.00	375000.00	0.0008
298.00	400000.00	0.0008
323.00	10000.00	0.0011
323.00	20000.00	0.0011
323.00	30000.00	0.0011
323.00	40000.00	0.0011
323.00	50000.00	0.0010
323.00	75000.00	0.0010
323.00	100000.00	0.0010
323.00	125000.00	0.0010
323.00	150000.00	0.0009
323.00	175000.00	0.0009
323.00	200000.00	0.0009
323.00	225000.00	0.0009
323.00	250000.00	0.0009
323.00	275000.00	0.0009

323.00	300000.00	0.0009
323.00	325000.00	0.0009
323.00	350000.00	0.0009
323.00	375000.00	0.0009
323.00	400000.00	0.0008
348.00	10000.00	0.0012
348.00	20000.00	0.0012
348.00	30000.00	0.0011
348.00	40000.00	0.0011
348.00	50000.00	0.0011
348.00	75000.00	0.0010
348.00	100000.00	0.0010
348.00	125000.00	0.0010
348.00	150000.00	0.0010
348.00	175000.00	0.0010
348.00	200000.00	0.0009
348.00	225000.00	0.0009
348.00	250000.00	0.0009
348.00	275000.00	0.0009
348.00	300000.00	0.0009
348.00	325000.00	0.0009
348.00	350000.00	0.0009
348.00	375000.00	0.0009
348.00	400000.00	0.0009
373.00	10000.00	0.0013
373.00	20000.00	0.0012
373.00	30000.00	0.0012
373.00	40000.00	0.0012
373.00	50000.00	0.0011
373.00	75000.00	0.0011
373.00	100000.00	0.0010
373.00	125000.00	0.0010
373.00	150000.00	0.0010
373.00	175000.00	0.0010
373.00	200000.00	0.0010
373.00	225000.00	0.0009
373.00	250000.00	0.0009
373.00	275000.00	0.0009
373.00	300000.00	0.0009
373.00	325000.00	0.0009
373.00	350000.00	0.0009
373.00	375000.00	0.0009
373.00	400000.00	0.0009
423.00	10000.00	0.0017

423.00	20000.00	0.0015
423.00	30000.00	0.0013
423.00	40000.00	0.0013
423.00	50000.00	0.0012
423.00	75000.00	0.0012
423.00	100000.00	0.0011
423.00	125000.00	0.0011
423.00	150000.00	0.0010
423.00	175000.00	0.0010
423.00	200000.00	0.0010
423.00	225000.00	0.0010
423.00	250000.00	0.0010
423.00	275000.00	0.0010
423.00	300000.00	0.0009
423.00	325000.00	0.0009
423.00	350000.00	0.0009
423.00	375000.00	0.0009
423.00	400000.00	0.0009
473.00	10000.00	0.0045
473.00	20000.00	0.0019
473.00	30000.00	0.0016
473.00	40000.00	0.0014
473.00	50000.00	0.0014
473.00	75000.00	0.0013
473.00	100000.00	0.0012
473.00	125000.00	0.0011
473.00	150000.00	0.0011
473.00	175000.00	0.0011
473.00	200000.00	0.0010
473.00	225000.00	0.0010
473.00	250000.00	0.0010
473.00	275000.00	0.0010
473.00	300000.00	0.0010
473.00	325000.00	0.0010
473.00	350000.00	0.0009
473.00	375000.00	0.0009
473.00	400000.00	0.0009
523.00	10000.00	0.0064
523.00	20000.00	0.0026
523.00	30000.00	0.0019
523.00	40000.00	0.0017
523.00	50000.00	0.0015
523.00	75000.00	0.0013
523.00	100000.00	0.0013

523.00	125000.00	0.0012
523.00	150000.00	0.0012
523.00	175000.00	0.0011
523.00	200000.00	0.0011
523.00	225000.00	0.0011
523.00	250000.00	0.0010
523.00	275000.00	0.0010
523.00	300000.00	0.0010
523.00	325000.00	0.0010
523.00	350000.00	0.0010
523.00	375000.00	0.0010
523.00	400000.00	0.0009
573.00	10000.00	0.0079
573.00	20000.00	0.0034
573.00	30000.00	0.0023
573.00	40000.00	0.0019
573.00	50000.00	0.0017
573.00	75000.00	0.0015
573.00	100000.00	0.0013
573.00	125000.00	0.0013
573.00	150000.00	0.0012
573.00	175000.00	0.0012
573.00	200000.00	0.0011
573.00	225000.00	0.0011
573.00	250000.00	0.0011
573.00	275000.00	0.0011
573.00	300000.00	0.0010
573.00	325000.00	0.0010
573.00	350000.00	0.0010
573.00	375000.00	0.0010
573.00	400000.00	0.0010

Reference *https://www.doi.org/10.1021/je060117o*

Sources

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Pressure-Volume-Temperature Properties of Methyl Chloride at High Pressures and Temperatures:	https://www.doi.org/10.1021/je060117o

Legend:

affp:	Proton affinity
basg:	Gas basicity
chg:	Standard gas 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
hsubt:	Enthalpy of sublimation 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
pt:	Triple Point Pressure
pvap:	Vapor pressure
rhoc:	Critical density
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
svapt:	Entropy of vaporization at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

vols: Specific Volume