Propane, 1,2-dichloro-

Other names:	1,2-Dichloropropane
	Bichlorure de propylene
	CH3CHClCH2Cl
	Dichloropropane
	Dwuchloropropan
	ENT 15,406
	NCI-C55141
	NSC 1237
	Propylene chloride
	Propylene dichloride
	R 270da
	Rcra waste number U083
	«alpha»,«beta»-dichloropropane
	Â«alphaÂ»,Â«betaÂ»-dichloropropane
Inchi:	InChI=1S/C3H6Cl2/c1-3(5)2-4/h3H,2H2,1H3
InchiKey:	KNKRKFALVUDBJE-UHFFFAOYSA-N
Formula:	C3H6Cl2
SMILES:	CC(Cl)CCl
Mol. weight [g/mol]:	112.99
CAS:	78-87-5

Physical Properties

Property code	Value	Unit	Source
af	0.2400		KDB
chl	-1883.20 ± 8.40	kJ/mol	NIST Webbook
dm	1.90	debye	KDB
gf	-83.15	kJ/mol	KDB
hf	-166.00	kJ/mol	KDB
hf	-162.80 ± 1.20	kJ/mol	NIST Webbook
hfus	8.40	kJ/mol	Joback Method
hvap	36.30	kJ/mol	NIST Webbook
hvap	38.40 ± 0.30	kJ/mol	NIST Webbook
hvap	36.20 ± 0.10	kJ/mol	NIST Webbook
hvap	36.30 ± 0.50	kJ/mol	NIST Webbook
hvap	36.10 ± 0.10	kJ/mol	NIST Webbook
ie	10.80 ± 0.10	eV	NIST Webbook
ie	11.06	eV	NIST Webbook

ie	10.87 ± 0.05	eV	NIST Webbook
ie	10.73	eV	NIST Webbook
ie	10.73	eV	NIST Webbook
log10ws	-1.60		Estimated Solubility Method
log10ws	-1.60		Aqueous Solubility Prediction Method
logp	1.852		Crippen Method
mcvol	77.610	ml/mol	McGowan Method
pc	4450.00	kPa	KDB
pc	4650.00 ± 150.00	kPa	NIST Webbook
rhoc	390.03 ± 14.69	kg/m3	NIST Webbook
rinpol	679.00		NIST Webbook
rinpol	670.00		NIST Webbook
rinpol	703.00		NIST Webbook
rinpol	691.00		NIST Webbook
rinpol	695.00		NIST Webbook
rinpol	691.00		NIST Webbook
rinpol	684.00		NIST Webbook
rinpol	691.00		NIST Webbook
rinpol	684.00		NIST Webbook
rinpol	688.00		NIST Webbook
rinpol	667.00		NIST Webbook
rinpol	688.00		NIST Webbook
rinpol	684.00		NIST Webbook
rinpol	700.00		NIST Webbook
rinpol	672.00		NIST Webbook
rinpol	674.00		NIST Webbook
rinpol	688.00		NIST Webbook
ripol	1044.00		NIST Webbook
ripol	1058.00		NIST Webbook
tb	370.55 ± 0.50	K	NIST Webbook
tb	369.97 ± 0.40	K	NIST Webbook
tb	374.65 ± 6.00	K	NIST Webbook
tb	368.80 ± 2.50	K	NIST Webbook
tb	369.50	K	KDB
tb	369.60	K	NIST Webbook
tb	368.86 ± 0.20	K	NIST Webbook
tb	369.55	K	NIST Webbook
tb	369.15 ± 2.00	K	NIST Webbook
tb	369.15 ± 2.00	K	NIST Webbook
tb	369.95 ± 0.50	K	NIST Webbook
tb	371.15 ± 6.00	K	NIST Webbook
tb	369.15 ± 1.00	K	NIST Webbook
tb	369.30 ± 0.50	K	NIST Webbook

tb	369.70 ± 0.30	K	NIST Webbook
tb	369.35 ± 0.07	K	NIST Webbook
tb	371.15 ± 0.70	K	NIST Webbook
tb	369.95 ± 0.60	K	NIST Webbook
tb	370.20 ± 1.00	K	NIST Webbook
tb	369.95 ± 0.50	K	NIST Webbook
tb	368.75 ± 0.60	K	NIST Webbook
tb	370.65 ± 2.00	K	NIST Webbook
tb	369.95 ± 0.50	K	NIST Webbook
tb	369.65 ± 0.40	K	NIST Webbook
tc	578.00 ± 3.00	K	NIST Webbook
tc	577.00	K	KDB
tf	172.73 ± 0.05	K	NIST Webbook
tf	172.62 ± 0.02	K	NIST Webbook
tf	172.75	K	NIST Webbook
tf	172.70	K	KDB
vc	0.226	m3/kmol	KDB
zc	0.2096310		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	137.54	J/mol×K	498.18	Joback Method
cpg	142.30	J/mol×K	529.32	Joback Method
cpg	121.79	J/mol×K	404.75	Joback Method
cpg	127.29	J/mol×K	435.89	Joback Method
cpg	132.53	J/mol×K	467.03	Joback Method
cpg	110.03	J/mol×K	342.46	Joback Method
cpg	116.04	J/mol×K	373.60	Joback Method
cpl	155.15	J/mol×K	288.72	Heat capacities of selected chlorohydrocarbons
cpl	156.81	J/mol×K	298.93	Heat capacities of selected chlorohydrocarbons
cpl	156.64	J/mol×K	298.93	Heat capacities of selected chlorohydrocarbons
cpl	155.40	J/mol×K	288.72	Heat capacities of selected chlorohydrocarbons
cpl	153.90	J/mol×K	278.51	Heat capacities of selected chlorohydrocarbons

cpl	159.39	J/mol×K	319.35	Heat capacities of selected chlorohydrocarbons
cpl	159.22	J/mol×K	319.35	Heat capacities of selected chlorohydrocarbons
cpl	161.05	J/mol×K	329.56	Heat capacities of selected chlorohydrocarbons
cpl	161.22	J/mol×K	329.56	Heat capacities of selected chlorohydrocarbons
cpl	162.80	J/mol×K	339.77	Heat capacities of selected chlorohydrocarbons
cpl	162.80	J/mol×K	339.77	Heat capacities of selected chlorohydrocarbons
cpl	154.40	J/mol×K	298.00	NIST Webbook
cpl	154.15	J/mol×K	278.51	Heat capacities of selected chlorohydrocarbons
cpl	152.99	J/mol×K	268.30	Heat capacities of selected chlorohydrocarbons
cpl	153.32	J/mol×K	268.30	Heat capacities of selected chlorohydrocarbons
cpl	157.73	J/mol×K	309.14	Heat capacities of selected chlorohydrocarbons
cpl	158.06	J/mol×K	309.14	Heat capacities of selected chlorohydrocarbons
dvisc	0.0004402	Pa×s	313.45	Joback Method
dvisc	0.0003384	Pa×s	342.46	Joback Method
dvisc	0.0063844	Pa×s	168.41	Joback Method
dvisc	0.0027307	Pa×s	197.42	Joback Method
dvisc	0.0014519	Pa×s	226.43	Joback Method
dvisc	0.0008911	Pa×s	255.44	Joback Method
dvisc	0.0006042	Pa×s	284.44	Joback Method
hfust	6.40	kJ/mol	172.70	NIST Webbook
hfust	6.40	kJ/mol	172.70	NIST Webbook
hvapt	34.30	kJ/mol	330.50	NIST Webbook
hvapt	31.38	kJ/mol	369.50	KDB
hvapt	34.70	kJ/mol	345.00	NIST Webbook
hvapt	39.40	kJ/mol	306.00	NIST Webbook

pvap	30.14	kPa	333.15	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
pvap	61.07	kPa	353.15	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
rfi	1.43656		298.15	Excess molar volumes and excess molar enthalpies for binary mixtures of 1,2-dichloropropane with methyl ethanoate, methyl propanoate, and methyl butanoate at T = 298.15K
rfi	1.43653		298.15	Excess molar volumes and excess molar enthalpies of binary mixtures for 1,2-dichloropropane + 2-alkoxyethanol acetates at 298.15K

rfi	1.43830		293.10	Vapor-Liquid Equilibria of Selected Components in Propylene Oxide Production
rfi	1.43656		298.15	Excess molar volumes and excess molar enthalpies of the binary mixtures of 1,2-dichloropropane with di- and triethylene glycol mono-alkyl ethers at T=298.15K
rhol	1149.10	kg/m3	298.15	Speed of sound as a function of temperature and pressure for propane derivatives
rhol	1150.00	kg/m3	293.00	KDB
srf	0.03	N/m	293.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45124e+01
Coeff. B	-3.33468e+03
Coeff. C	-3.29610e+01
Temperature range (K), min.	267.39
Temperature range (K), max.	395.39

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	5.79698e+01
Coeff. B	-5.98019e+03
Coeff. C	-6.37968e+00
Coeff. D	4.07190e-06
Temperature range (K), min.	172.71
Temperature range (K), max.	577.00

Sources

The Critical Temperatures of a Number of (i) (Chloroalkane (C3 C4) + Hydrocarbon (C6 C7)) Binary Mixtures and (ii) (Aromatic Halocarbon (Chlorobenzene + Fluorobenzene, or 1,2-Dichlorobenzene, or 1,3-Dichlorobenzene) + Alkane (C8)) Binary Mixtures:	https://www.doi.org/10.1021/acs.jced.7b00191
Abraham model correlations for describing the thermodynamic properties of solute transfer into pentyl acetate based on headspace chromatographic and solubility measurements:	https://www.doi.org/10.1016/j.jct.2018.05.003
Vapor-Liquid Equilibria of Selected Components in Propylene Oxide Production:	https://www.doi.org/10.1021/je800122x
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Abraham model linear free energy relationships for describing the partitioning and solubility behavior of nonelectrolyte organic solutes dissolved in pyridine at 298.15 K:	https://www.doi.org/10.1016/j.fluid.2016.10.009
Determination of Henry's Law Constants Using Internal Standards with Benchmark Values:	https://www.doi.org/10.1021/je3010535
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1588
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1588
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:	https://www.doi.org/10.1021/je050317k
Excess molar volumes and excess molar enthalpies for binary mixtures of 1,2-dichloropropane with methyl ethanoate, methyl propanoate, and methyl butanoate at 298.15K:	https://www.doi.org/10.1016/j.fluid.2011.01.005
Heat capacities of selected chlorohydrocarbons:	https://www.doi.org/10.1016/j.fluid.2012.09.001
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C78875&Units=SI
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
Excess molar volumes and excess molar enthalpies of the binary mixtures of 1,2-dichloropropane with di- and triethylene glycol mono-alkyl ethers at T=298.15K:	https://www.doi.org/10.1016/j.fluid.2009.06.018
Speed of sound as a function of temperature and pressure for propane derivatives:	https://www.doi.org/10.1016/j.jct.2016.12.016
Excess molar volumes and excess molar enthalpies of binary mixtures for 1,2-dichloropropane + 2-alkoxyethanol acetates at 298.15K:	https://www.doi.org/10.1016/j.tca.2008.02.008

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
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
rfi:	Refractive Index
rhoc:	Critical density
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility

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