

Propane, 1,1-dichloro-

Other names:	1,1-Dichloropropane PROPYLIDENE CHLORIDE
Inchi:	InChI=1S/C3H6Cl2/c1-2-3(4)5/h3H,2H2,1H3
InchiKey:	WIHMGGWNMISDNJ-UHFFFAOYSA-N
Formula:	C3H6Cl2
SMILES:	CCC(Cl)Cl
Mol. weight [g/mol]:	112.99
CAS:	78-99-9

Physical Properties

Property code	Value	Unit	Source
gf	-51.92	kJ/mol	Joback Method
hf	-142.01	kJ/mol	Joback Method
hfus	8.40	kJ/mol	Joback Method
hvap	35.20 ± 0.40	kJ/mol	NIST Webbook
hvap	35.20	kJ/mol	NIST Webbook
log10ws	-1.99		Crippen Method
logp	2.200		Crippen Method
mcvol	77.610	ml/mol	McGowan Method
pc	4046.64	kPa	Joback Method
rinpol	668.00		NIST Webbook
rinpol	668.00		NIST Webbook
rinpol	668.00		NIST Webbook
rinpol	686.00		NIST Webbook
rinpol	686.00		NIST Webbook
tb	363.15 ± 1.00	K	NIST Webbook
tb	360.00 ± 2.00	K	NIST Webbook
tb	351.00 ± 3.00	K	NIST Webbook
tb	361.25 ± 0.50	K	NIST Webbook
tb	361.30	K	NIST Webbook
tc	529.32	K	Joback Method
tf	168.41	K	Joback Method
vc	0.295	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	110.03	J/mol×K	342.46	Joback Method
cpg	142.30	J/mol×K	529.32	Joback Method
cpg	137.54	J/mol×K	498.18	Joback Method
cpg	132.53	J/mol×K	467.03	Joback Method
cpg	127.29	J/mol×K	435.89	Joback Method
cpg	121.79	J/mol×K	404.75	Joback Method
cpg	116.04	J/mol×K	373.60	Joback Method
cpl	159.31	J/mol×K	339.77	Heat capacities of selected chlorohydrocarbons
cpl	155.56	J/mol×K	319.35	Heat capacities of selected chlorohydrocarbons
cpl	157.23	J/mol×K	329.56	Heat capacities of selected chlorohydrocarbons
cpl	157.31	J/mol×K	329.56	Heat capacities of selected chlorohydrocarbons
cpl	157.64	J/mol×K	329.56	Heat capacities of selected chlorohydrocarbons
cpl	158.97	J/mol×K	339.77	Heat capacities of selected chlorohydrocarbons
cpl	159.06	J/mol×K	339.77	Heat capacities of selected chlorohydrocarbons
cpl	148.83	J/mol×K	268.30	Heat capacities of selected chlorohydrocarbons
cpl	149.66	J/mol×K	268.30	Heat capacities of selected chlorohydrocarbons
cpl	149.49	J/mol×K	268.31	Heat capacities of selected chlorohydrocarbons
cpl	150.33	J/mol×K	278.51	Heat capacities of selected chlorohydrocarbons
cpl	150.24	J/mol×K	278.51	Heat capacities of selected chlorohydrocarbons
cpl	155.90	J/mol×K	319.35	Heat capacities of selected chlorohydrocarbons

cpl	151.82	J/mol×K	288.72	Heat capacities of selected chlorohydrocarbons
cpl	151.99	J/mol×K	288.72	Heat capacities of selected chlorohydrocarbons
cpl	152.40	J/mol×K	288.72	Heat capacities of selected chlorohydrocarbons
cpl	152.82	J/mol×K	298.93	Heat capacities of selected chlorohydrocarbons
cpl	152.82	J/mol×K	298.93	Heat capacities of selected chlorohydrocarbons
cpl	153.65	J/mol×K	298.93	Heat capacities of selected chlorohydrocarbons
cpl	155.23	J/mol×K	309.14	Heat capacities of selected chlorohydrocarbons
cpl	154.57	J/mol×K	309.14	Heat capacities of selected chlorohydrocarbons
cpl	154.15	J/mol×K	309.14	Heat capacities of selected chlorohydrocarbons
cpl	149.99	J/mol×K	278.51	Heat capacities of selected chlorohydrocarbons
cpl	157.73	J/mol×K	319.35	Heat capacities of selected chlorohydrocarbons
dvisc	0.0003384	Pa×s	342.46	Joback Method
dvisc	0.0004402	Pa×s	313.45	Joback Method
dvisc	0.0006042	Pa×s	284.44	Joback Method
dvisc	0.0008911	Pa×s	255.44	Joback Method
dvisc	0.0014519	Pa×s	226.43	Joback Method
dvisc	0.0027307	Pa×s	197.42	Joback Method
dvisc	0.0063844	Pa×s	168.41	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.43093e+01
Coeff. B	-3.07582e+03
Coeff. C	-4.39110e+01

Temperature range (K), min.	263.27
Temperature range (K), max.	385.75

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	7.65115e+01
Coeff. B	-6.65889e+03
Coeff. C	-9.22649e+00
Coeff. D	6.74782e-06
Temperature range (K), min.	200.00
Temperature range (K), max.	560.00

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C78999&Units=SI
Heat capacities of selected chlorohydrocarbons:	https://www.doi.org/10.1016/j.fluid.2012.09.001
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB:	https://www.thermo.com/files/research/kdb/mol/mol1587.mol
KDB Vapor Pressure Data:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1587
Crippen Method:	https://www.chemed.com/doc/models/crippen_log10ws
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp _g :	Ideal gas heat capacity
cp _l :	Liquid phase heat capacity
dv _{isc} :	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hf _{us} :	Enthalpy of fusion at standard conditions
hv _{ap} :	Enthalpy of vaporization at standard conditions
log ₁₀ ws:	Log10 of Water solubility in mol/l
log _p :	Octanol/Water partition coefficient
mc _{vol} :	McGowan's characteristic volume

pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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