

Propane, 2-chloro-

Other names:	2-Chloropropane 2-Propyl chloride CHLORODIMETHYLMETHANE ISOPROPYL CHLORIDE Isoprid Narcosop SEC-PROPYL CHLORIDE UN 2356 iso-C3H7Cl
Inchi:	InChI=1S/C3H7Cl/c1-3(2)4/h3H,1-2H3
InchiKey:	ULYZAYCEDJDHCC-UHFFFAOYSA-N
Formula:	C3H7Cl
SMILES:	CC(C)Cl
Mol. weight [g/mol]:	78.54
CAS:	75-29-6

Physical Properties

Property code	Value	Unit	Source
af	0.2320		KDB
chg	-2059.60 ± 0.79	kJ/mol	NIST Webbook
chl	-2028.40 ± 8.40	kJ/mol	NIST Webbook
dm	2.10	debye	KDB
gf	-62.55	kJ/mol	KDB
hf	-146.50	kJ/mol	KDB
hfus	4.20	kJ/mol	Joback Method
hvap	27.60	kJ/mol	NIST Webbook
ie	10.78	eV	NIST Webbook
ie	10.81	eV	NIST Webbook
ie	10.75	eV	NIST Webbook
ie	10.77 ± 0.03	eV	NIST Webbook
ie	11.00 ± 0.10	eV	NIST Webbook
ie	10.78 ± 0.02	eV	NIST Webbook
ie	10.78 ± 0.02	eV	NIST Webbook
log10ws	-1.41		Aqueous Solubility Prediction Method
log10ws	-1.41		Estimated Solubility Method

logp	1.634		Crippen Method
mcvol	65.370	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=2)		KDB
nfpas	%!d(float64=1)		KDB
pc	4720.00	kPa	KDB
rinpol	479.00		NIST Webbook
rinpol	488.00		NIST Webbook
rinpol	480.00		NIST Webbook
rinpol	491.40		NIST Webbook
rinpol	491.00		NIST Webbook
rinpol	507.00		NIST Webbook
rinpol	477.00		NIST Webbook
rinpol	496.00		NIST Webbook
rinpol	496.00		NIST Webbook
rinpol	496.00		NIST Webbook
rinpol	496.00		NIST Webbook
rinpol	496.00		NIST Webbook
rinpol	496.00		NIST Webbook
rinpol	495.00		NIST Webbook
rinpol	478.00		NIST Webbook
rinpol	477.00		NIST Webbook
rinpol	475.00		NIST Webbook
rinpol	490.00		NIST Webbook
rinpol	490.72		NIST Webbook
tb	308.00	K	KDB
tc	485.00	K	KDB
tf	156.15 ± 0.50	K	NIST Webbook
tf	155.97 ± 0.02	K	NIST Webbook
tf	155.85	K	Aqueous Solubility Prediction Method
tf	156.00	K	KDB
vc	0.230	m ³ /kmol	KDB
zc	0.2692100		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	117.36	J/mol×K	451.69	Joback Method
cpg	122.37	J/mol×K	481.02	Joback Method
cpg	89.12	J/mol×K	305.03	Joback Method

cpg	95.20	J/molxK	334.36	Joback Method
cpg	101.06	J/molxK	363.69	Joback Method
cpg	106.71	J/molxK	393.02	Joback Method
cpg	112.14	J/molxK	422.35	Joback Method
dvisc	0.0002551	Paxs	305.03	Joback Method
dvisc	0.0003319	Paxs	277.27	Joback Method
dvisc	0.0060246	Paxs	138.49	Joback Method
dvisc	0.0022908	Paxs	166.25	Joback Method
dvisc	0.0011487	Paxs	194.00	Joback Method
dvisc	0.0006847	Paxs	221.76	Joback Method
dvisc	0.0004579	Paxs	249.52	Joback Method
hfust	7.39	kJ/mol	156.00	NIST Webbook
hfust	7.39	kJ/mol	156.00	NIST Webbook
hvapt	27.30	kJ/mol	288.00	NIST Webbook
hvapt	27.20 ± 0.84	kJ/mol	307.00	NIST Webbook
hvapt	26.28	kJ/mol	308.00	KDB
hvapt	30.20	kJ/mol	274.50	NIST Webbook
hvapt	30.60	kJ/mol	251.50	NIST Webbook
rhoI	862.00	kg/m3	293.00	KDB
srf	0.02	N/m	293.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.38739e+01
Coeff. B	-2.34111e+03
Coeff. C	-5.50590e+01
Temperature range (K), min.	227.37
Temperature range (K), max.	329.63

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	1.93760e+02
Coeff. B	-9.55303e+03
Coeff. C	-2.82260e+01
Coeff. D	3.79510e-05
Temperature range (K), min.	155.97

Datasets

Mass density, kg/m³

Pressure, kPa - Liquid	Temperature, K - Liquid	Mass density, kg/m ³ - Liquid
100.00	283.15	875.68
100.00	288.15	869.67
100.00	293.15	862.78
100.00	298.15	856.08
100.00	303.15	849.46
100.00	308.15	843.35
2000.00	283.15	878.08
2000.00	288.15	872.23
2000.00	293.15	865.38
2000.00	298.15	858.81
2000.00	303.15	852.23
2000.00	308.15	846.3
5000.00	283.15	881.8
5000.00	288.15	876.01
5000.00	293.15	869.35
5000.00	298.15	862.94
5000.00	303.15	856.56
5000.00	308.15	850.7
7000.00	283.15	884.04
7000.00	288.15	878.42
7000.00	293.15	871.96
7000.00	298.15	865.59
7000.00	303.15	859.35
7000.00	308.15	853.65
10000.00	283.15	887.49
10000.00	288.15	881.91
10000.00	293.15	875.7
10000.00	298.15	869.47
10000.00	303.15	863.41
10000.00	308.15	857.84
20000.00	283.15	898.23
20000.00	288.15	893.01

20000.00	293.15	887.07
20000.00	298.15	881.27
20000.00	303.15	875.73
20000.00	308.15	870.52
30000.00	283.15	907.91
30000.00	288.15	903.04
30000.00	293.15	897.36
30000.00	298.15	891.91
30000.00	303.15	886.62
30000.00	308.15	881.67
40000.00	283.15	916.87
40000.00	288.15	912.1
40000.00	293.15	906.64
40000.00	298.15	901.57
40000.00	303.15	896.48
40000.00	308.15	891.77
50000.00	283.15	925.04
50000.00	288.15	920.44
50000.00	293.15	915.26
50000.00	298.15	910.44
50000.00	303.15	905.52
50000.00	308.15	901.08
60000.00	283.15	932.67
60000.00	288.15	928.22
60000.00	293.15	923.28
60000.00	298.15	918.62
60000.00	303.15	913.87
60000.00	308.15	909.58
65000.00	283.15	936.33
65000.00	288.15	931.95
65000.00	293.15	927.07
65000.00	298.15	922.46
65000.00	303.15	917.82
65000.00	308.15	913.53

Reference

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Sources

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<http://webbook.nist.gov/cgi/cbook.cgi?ID=C75296&Units=SI>

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Volumetric Properties of Short-Chain Chloroalkanes:	https://www.doi.org/10.1021/je3003805
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1595.mol
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1595
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

af:	Acentric Factor
chg:	Standard gas enthalpy of combustion
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas 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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
nfpas:	NFPA Safety Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rho:	Liquid Density
rinpol:	Non-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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