Allyl chloride

Other names:	1-CHLORO-2-PROPENE
	1-Chloropropene-2
	1-Propene, 3-chloro-
	2-PROPENYL CHLORIDE
	3-Chloro-1-propene
	3-Chloro-1-propylene
	3-Chloropropene
	3-Chloropropene-1
	3-Chloropropylene
	3-Chlorpropen
	3-chloropropene (allyl chloride)
	Allile(cloruro di)
	Allylchlorid
	Allyle(chlorure d')
	CH2=CHCH2Cl
	Chlorallylene
	Chloroallylene
	NCI-C04615
	NSC 20939
	Propene, 3-chloro-
	UN 1100
	«alpha»-Chloropropylene
	Â«alphaÂ»-Chloropropylene
Inchi:	InChI=1S/C3H5Cl/c1-2-3-4/h2H,1,3H2
InchiKey:	OSDWBNJEKMUWAV-UHFFFAOYSA-N
Formula:	C3H5Cl
SMILES:	C=CCCl
Mol. weight [g/mol]:	76.53
CAS:	107-05-1

Physical Properties

Property code	Value	Unit	Source
gf	50.29	kJ/mol	Joback Method
hf	-5.60	kJ/mol	NIST Webbook
hfus	6.44	kJ/mol	Joback Method
hvap	29.90	kJ/mol	NIST Webbook

ie	10.04 ± 0.01	eV	NIST Webbook
ie	10.05	eV	NIST Webbook
ie	10.05	eV	NIST Webbook
ie	10.34	eV	NIST Webbook
ie	9.90	eV	NIST Webbook
ie	10.05	eV	NIST Webbook
ie	10.05 ± 0.01	eV	NIST Webbook
ie	10.20	eV	NIST Webbook
ie	10.34	eV	NIST Webbook
log10ws	-1.36		Aqueous Solubility Prediction Method
logp	1.411		Crippen Method
mcvol	61.070	ml/mol	McGowan Method
pc	4438.52	kPa	Joback Method
rinpol	526.00		NIST Webbook
rinpol	526.00		NIST Webbook
rinpol	498.00		NIST Webbook
rinpol	526.00		NIST Webbook
rinpol	500.00		NIST Webbook
rinpol	516.00		NIST Webbook
rinpol	495.00		NIST Webbook
tb	318.30 ± 0.30	K	NIST Webbook
tb	318.90 ± 0.50	K	NIST Webbook
tb	318.15 ± 0.30	K	NIST Webbook
tb	317.75 ± 0.30	K	NIST Webbook
tb	318.30 ± 0.40	K	NIST Webbook
tb	318.00	K	NIST Webbook
tb	318.20	K	NIST Webbook
tb	318.30	K	KDB
tb	317.45 ± 0.50	K	NIST Webbook
tb	318.25 ± 0.20	K	NIST Webbook
tb	318.30 ± 0.50	K	NIST Webbook
tb	318.60 ± 0.50	K	NIST Webbook
tb	318.30 ± 0.30	K	NIST Webbook
tc	514.00	K	KDB
tf	136.75 ± 0.40	K	NIST Webbook
tf	138.65 ± 0.50	K	NIST Webbook
tf	138.53	K	Aqueous Solubility Prediction Method
tf	138.60	K	KDB
vc	0.234	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	105.54	J/mol×K	477.44	Joback Method
cpg	83.18	J/mol×K	331.37	Joback Method
cpg	88.07	J/mol×K	360.58	Joback Method
cpg	92.74	J/mol×K	389.80	Joback Method
cpg	97.21	J/mol×K	419.01	Joback Method
cpg	101.47	J/mol×K	448.23	Joback Method
cpg	78.06	J/mol×K	302.15	Joback Method
cpl	125.10	J/mol×K	298.00	NIST Webbook
dvisc	0.0002930	Pa×s	277.08	Joback Method
dvisc	0.0003766	Pa×s	252.01	Joback Method
dvisc	0.0005116	Pa×s	226.94	Joback Method
dvisc	0.0007501	Pa×s	201.87	Joback Method
dvisc	0.0012256	Pa×s	176.80	Joback Method
dvisc	0.0002377	Pa×s	302.15	Joback Method
dvisc	0.0023556	Pa×s	151.73	Joback Method
hvapt	30.00	kJ/mol	301.50	NIST Webbook
hvapt	33.10	kJ/mol	260.50	NIST Webbook
pvap	75.00	kPa	308.19	Vapor Liquid Equilibria of the Binary System 1,5-Hexadiene + Allyl Chloride
pvap	228.00	kPa	343.12	Vapor Liquid Equilibria of the Binary System 1,5-Hexadiene + Allyl Chloride
pvap	301.00	kPa	353.05	Vapor Liquid Equilibria of the Binary System 1,5-Hexadiene + Allyl Chloride
pvap	90.00	kPa	313.35	Vapor Liquid Equilibria of the Binary System 1,5-Hexadiene + Allyl Chloride
pvap	126.00	kPa	323.75	Vapor Liquid Equilibria of the Binary System 1,5-Hexadiene + Allyl Chloride
pvap	233.00	kPa	343.83	Vapor Liquid Equilibria of the Binary System 1,5-Hexadiene + Allyl Chloride

pvap	389.00	kPa	363.03	Vapor Liquid Equilibria of the Binary System 1,5-Hexadiene + Allyl Chloride
pvap	454.00	kPa	369.15	Vapor Liquid Equilibria of the Binary System 1,5-Hexadiene + Allyl Chloride
pvap	173.00	kPa	333.47	Vapor Liquid Equilibria of the Binary System 1,5-Hexadiene + Allyl Chloride
pvap	125.00	kPa	323.13	Vapor Liquid Equilibria of the Binary System 1,5-Hexadiene + Allyl Chloride
pvap	55.00	kPa	298.88	Vapor Liquid Equilibria of the Binary System 1,5-Hexadiene + Allyl Chloride
pvap	489.25	kPa	373.10	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	164.65	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	126.00	kPa	323.19	Vapor Liquid Equilibria of the Binary System 1,5-Hexadiene + Allyl Chloride
pvap	294.00	kPa	352.30	Vapor Liquid Equilibria of the Binary System 1,5-Hexadiene + Allyl Chloride
rfi	1.41550		293.00	Liquid-Liquid Equilibria for the Epichlorohydrin + Water + Methanol and Allyl Chloride + Water + Methanol Systems

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38315e+01
Coeff. B	-2.52007e+03
Coeff. C	-4.46710e+01
Temperature range (K), min.	230.74
Temperature range (K), max.	514.15

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	3.00180e+01
Coeff. B	-4.11134e+03
Coeff. C	-2.16341e+00
Coeff. D	-3.89227e-07
Temperature range (K), min.	138.65
Temperature range (K), max.	514.15

Sources

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
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1740.mol
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C107051&Units=SI
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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Determination of Henry's Law Constants Using Internal Standards with Benchmark Values:	https://www.doi.org/10.1021/je3010535
Liquid-Liquid Equilibria for the Epichlorohydrin + Water + Methanol and Allyl Chloride + Water + Methanol Systems:	https://www.doi.org/10.1021/je034018b
Vapor-Liquid Equilibria of the Binary System 1,5-Hexadiene + Allyl Chloride:	https://www.doi.org/10.1021/je400755x
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1740

Legend

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
hfus:	Enthalpy of fusion at standard conditions
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
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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