1-Propene, 2-chloro-

Other names:	2-CHLOROPROPYLENE
	2-Chloro-1-propene
	2-Chloropropene
	2-Chloropropene-1
	BETA-CHLOROPROPENE
	ISOPROPENYL CHLORIDE
	Propene, 2-chloro-
	UN 2456
	«beta»-Chloropropene
	«beta»-Chloropropylene
	Â«betaÂ»-Chloropropene
	Â«betaÂ»-Chloropropylene
Inchi:	InChI=1S/C3H5Cl/c1-3(2)4/h1H2,2H3
InchiKey:	PNLQPWWBHXMFCA-UHFFFAOYSA-N
Formula:	C3H5Cl
SMILES:	C=C(C)Cl
Mol. weight [g/mol]:	76.53
CAS:	557-98-2

Physical Properties

Property code	Value	Unit	Source
gf	41.74	kJ/mol	Joback Method
hf	-24.70	kJ/mol	NIST Webbook
hfus	5.13	kJ/mol	Joback Method
hvap	26.07	kJ/mol	Joback Method
log10ws	-1.58		Crippen Method
logp	1.759		Crippen Method
mcvol	61.070	ml/mol	McGowan Method
pc	4468.24	kPa	Joback Method
rinpol	470.00		NIST Webbook
rinpol	470.00		NIST Webbook
rinpol	470.00		NIST Webbook
tb	302.03	K	Joback Method
tc	481.19	K	Joback Method
tf	135.80 ± 0.40	K	NIST Webbook
vc	0.234	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	101.88	J/mol×K	451.33	Joback Method
cpg	78.16	J/mol×K	302.03	Joback Method
cpg	83.36	J/mol×K	331.89	Joback Method
cpg	88.32	J/mol×K	361.75	Joback Method
cpg	93.06	J/mol×K	391.61	Joback Method
cpg	97.58	J/mol×K	421.47	Joback Method
cpg	105.98	J/mol×K	481.19	Joback Method
hvapt	28.00	kJ/mol	278.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38889e+01
Coeff. B	-2.38388e+03
Coeff. C	-3.85560e+01
Temperature range (K), min.	213.82
Temperature range (K), max.	316.62

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	3.96868e+01
Coeff. B	-4.09231e+03
Coeff. C	-3.77471e+00
Coeff. D	2.60482e-06
Temperature range (K), min.	135.75
Temperature range (K), max.	478.00

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C557982&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1739
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1739.mol

Legend

cpg:	Ideal gas heat capacity
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	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