trans-1-Chloropropene

Other names:	(E)-1-Chloro-1-propene
	(E)-1-Propene, 1-chloro
	1-Propene, 1-chloro-, (E)-
	Propene, 1-chloro-, (E)-
	trans-1-Chloro-1-Propene
	trans-1-Propenyl chloride
Inchi:	InChI=1S/C3H5Cl/c1-2-3-4/h2-3H,1H3/b3-2+
InchiKey:	OWXJKYNZGFSVRC-NSCUHMNNSA-N
Formula:	C3H5Cl
SMILES:	CC=CCl
Mol. weight [g/mol]:	76.53
CAS:	16136-85-9

Physical Properties

Property code	Value	Unit	Source
gf	42.67	kJ/mol	Joback Method
hf	-12.00	kJ/mol	NIST Webbook
hfus	7.92	kJ/mol	Joback Method
hvap	26.62	kJ/mol	Joback Method
log10ws	-1.58		Crippen Method
logp	1.759		Crippen Method
mcvol	61.070	ml/mol	McGowan Method
pc	4498.26	kPa	Joback Method
rinpol	510.00		NIST Webbook
rinpol	510.00		NIST Webbook
tb	310.60	K	NIST Webbook
tb	37.40 ± 0.50	K	NIST Webbook
tb	309.90 ± 1.00	K	NIST Webbook
tb	309.85 ± 1.00	K	NIST Webbook
tc	491.40	K	Joback Method
tf	148.41	K	Joback Method
vc	0.233	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	100.54	J/mol×K	461.11	Joback Method
cpg	104.74	J/mol×K	491.40	Joback Method
cpg	75.64	J/mol×K	309.63	Joback Method
cpg	81.19	J/mol×K	339.93	Joback Method
cpg	86.44	J/mol×K	370.22	Joback Method
cpg	91.40	J/mol×K	400.52	Joback Method
cpg	96.10	J/mol×K	430.81	Joback Method
dvisc	0.0002055	Pa×s	309.63	Joback Method
dvisc	0.0002580	Pa×s	282.76	Joback Method
dvisc	0.0027616	Pa×s	148.41	Joback Method
dvisc	0.0012852	Pa×s	175.28	Joback Method
dvisc	0.0007330	Pa×s	202.15	Joback Method
dvisc	0.0004769	Pa×s	229.02	Joback Method
dvisc	0.0003396	Pa×s	255.89	Joback Method
hvapt	29.70	kJ/mol	292.00	NIST Webbook
hvapt	28.50	kJ/mol	308.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41161e+01
Coeff. B	-2.59220e+03
Coeff. C	-3.76730e+01
Temperature range (K), min.	225.13
Temperature range (K), max.	332.09

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C16136859&Units=SI

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

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas 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
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

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