

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	37.40 ± 0.50	K	NIST Webbook
tb	310.60	K	NIST Webbook
tb	309.85 ± 1.00	K	NIST Webbook
tb	309.90 ± 1.00	K	NIST Webbook
tc	491.40	K	Joback Method
tf	148.41	K	Joback Method
vc	0.233	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
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

McGowan Method:

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

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/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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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