

# 1-Propene, 3,3,3-trichloro-

<b>Other names:</b>	3,3,3-Dichloro-1-propene 3,3,3-Trichloro-1-propene 3,3,3-Trichloropropene CH <sub>2</sub> =CHCCl <sub>3</sub> Propene, 3,3,3-trichloro-
<b>Inchi:</b>	InChI=1S/C3H3Cl3/c1-2-3(4,5)6/h2H,1H2
<b>InchiKey:</b>	VKEIPALYOJMDAC-UHFFFAOYSA-N
<b>Formula:</b>	C <sub>3</sub> H <sub>3</sub> Cl <sub>3</sub>
<b>SMILES:</b>	C=CC(Cl)(Cl)Cl
<b>Mol. weight [g/mol]:</b>	145.41
<b>CAS:</b>	2233-00-3

## Physical Properties

Property code	Value	Unit	Source
gf	29.27	kJ/mol	Joback Method
hf	-35.79	kJ/mol	Joback Method
hfus	7.42	kJ/mol	Joback Method
hvap	33.46	kJ/mol	Joback Method
log10ws	-2.49		Crippen Method
logp	2.543		Crippen Method
mcvol	85.550	ml/mol	McGowan Method
pc	4130.29	kPa	Joback Method
tb	373.78	K	Joback Method
tc	583.74	K	Joback Method
tf	213.99	K	Joback Method
vc	0.321	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	118.61	J/mol×K	373.78	Joback Method
cpg	124.58	J/mol×K	408.77	Joback Method
cpg	129.99	J/mol×K	443.77	Joback Method
cpg	134.90	J/mol×K	478.76	Joback Method

cpg	139.33	J/molxK	513.75	Joback Method
cpg	143.33	J/molxK	548.74	Joback Method
cpg	146.93	J/molxK	583.74	Joback Method
dvisc	0.0058212	Paxs	213.99	Joback Method
dvisc	0.0029991	Paxs	240.62	Joback Method
dvisc	0.0017635	Paxs	267.25	Joback Method
dvisc	0.0011417	Paxs	293.88	Joback Method
dvisc	0.0007945	Paxs	320.52	Joback Method
dvisc	0.0005845	Paxs	347.15	Joback Method
dvisc	0.0004493	Paxs	373.78	Joback Method

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.34973e+01
Coeff. B	-3.08054e+03
Coeff. C	-4.89170e+01
Temperature range (K), min.	282.12
Temperature range (K), max.	425.24

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2233003&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2233003&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation

<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvac:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/81-265-8/1-Propene-3-3-3-trichloro.pdf>

Generated by Cheméo on 2024-04-26 09:05:03.721757809 +0000 UTC m=+16411552.642335121.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.