

# 1-Propene, 1,1,2-trichloro-

<b>Other names:</b>	1,1,2-Trichloro-1-propene 1,1,2-Trichloropropene Propene, 1,1,2-trichloro-
<b>Inchi:</b>	InChI=1S/C3H3Cl3/c1-2(4)3(5)6/h1H3
<b>InchiKey:</b>	LIPPKMMVZOHCIF-UHFFFAOYSA-N
<b>Formula:</b>	C3H3Cl3
<b>SMILES:</b>	CC(Cl)=C(Cl)Cl
<b>Mol. weight [g/mol]:</b>	145.41
<b>CAS:</b>	21400-25-9

## Physical Properties

Property code	Value	Unit	Source
gf	1.71	kJ/mol	Joback Method
hf	-54.83	kJ/mol	Joback Method
hfus	13.70	kJ/mol	Joback Method
hvap	35.55	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.892		Crippen Method
mcvol	85.550	ml/mol	McGowan Method
pc	4135.61	kPa	Joback Method
tb	384.25	K	Joback Method
tc	594.98	K	Joback Method
tf	180.33	K	Joback Method
vc	0.333	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	114.84	J/molxK	384.25	Joback Method
cpg	119.98	J/molxK	419.37	Joback Method
cpg	124.73	J/molxK	454.49	Joback Method
cpg	129.11	J/molxK	489.61	Joback Method
cpg	133.15	J/molxK	524.73	Joback Method
cpg	136.88	J/molxK	559.86	Joback Method

cpg

140.31

J/mol×K

594.98

Joback Method

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.37927e+01
Coeff. B	-3.17411e+03
Coeff. C	-4.98900e+01
Temperature range (K), min.	284.92
Temperature range (K), max.	424.14

## Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

Joback Method:

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

McGowan Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C21400259&Units=SI>

The Yaws Handbook of Vapor Pressure:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<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>hvap:</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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>tb:</b>	Normal Boiling Point Temperature

**tc:** Critical Temperature  
**tf:** Normal melting (fusion) point  
**vc:** Critical Volume

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