

# Propane, 1,1,2-trichloro-2-methyl-

<b>Inchi:</b>	InChI=1S/C4H7Cl3/c1-4(2,7)3(5)6/h3H,1-2H3
<b>InchiKey:</b>	FRRHZKFKOHHEJR-UHFFFAOYSA-N
<b>Formula:</b>	C4H7Cl3
<b>SMILES:</b>	CC(C)(Cl)C(Cl)Cl
<b>Mol. weight [g/mol]:</b>	161.46
<b>CAS:</b>	29559-52-2

## Physical Properties

Property code	Value	Unit	Source
gf	-52.59	kJ/mol	Joback Method
hf	-187.14	kJ/mol	Joback Method
hfus	7.77	kJ/mol	Joback Method
hvap	35.97	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	2.807		Crippen Method
mcvol	103.940	ml/mol	McGowan Method
pc	3517.91	kPa	Joback Method
rinpol	869.00		NIST Webbook
rinpol	869.00		NIST Webbook
tb	399.54	K	Joback Method
tc	608.09	K	Joback Method
tf	212.02	K	Joback Method
vc	0.390	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	165.86	J/mol×K	399.54	Joback Method
cpg	174.47	J/mol×K	434.30	Joback Method
cpg	182.46	J/mol×K	469.06	Joback Method
cpg	189.88	J/mol×K	503.81	Joback Method
cpg	196.74	J/mol×K	538.57	Joback Method
cpg	203.10	J/mol×K	573.33	Joback Method
cpg	208.98	J/mol×K	608.09	Joback Method

dvisc	0.0108227	Paxs	212.02	Joback Method
dvisc	0.0044160	Paxs	243.27	Joback Method
dvisc	0.0022098	Paxs	274.53	Joback Method
dvisc	0.0012740	Paxs	305.78	Joback Method
dvisc	0.0008134	Paxs	337.03	Joback Method
dvisc	0.0005605	Paxs	368.29	Joback Method
dvisc	0.0004093	Paxs	399.54	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>
<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=C29559522&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C29559522&amp;Units=SI</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>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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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