

# 2,4,5-Trichlorotoluene

<b>Other names:</b>	Benzene, 1,2,4-trichloro-5-methyl-Toluene, 2,4,5-trichloro-Benzene, 1-methyl-2,4,5-trichloro-
<b>Inchi:</b>	InChI=1S/C7H5Cl3/c1-4-2-6(9)7(10)3-5(4)8/h2-3H,1H3
<b>InchiKey:</b>	ZCXHZKNWIYVQNC-UHFFFAOYSA-N
<b>Formula:</b>	C7H5Cl3
<b>SMILES:</b>	Cc1cc(Cl)c(Cl)cc1Cl
<b>Mol. weight [g/mol]:</b>	195.47
<b>CAS:</b>	6639-30-1

## Physical Properties

Property code	Value	Unit	Source
gf	55.79	kJ/mol	Joback Method
hf	-32.91	kJ/mol	Joback Method
hfus	19.35	kJ/mol	Joback Method
hvap	48.59	kJ/mol	Joback Method
ie	8.80	eV	NIST Webbook
log10ws	-4.00		Crippen Method
logp	3.955		Crippen Method
mcvol	122.450	ml/mol	McGowan Method
pc	3399.94	kPa	Joback Method
tb	513.47	K	Joback Method
tc	749.79	K	Joback Method
tf	322.39	K	Joback Method
vc	0.467	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	207.21	J/molxK	513.47	Joback Method
cpg	215.47	J/molxK	552.86	Joback Method
cpg	223.21	J/molxK	592.24	Joback Method
cpg	230.46	J/molxK	631.63	Joback Method
cpg	237.23	J/molxK	671.02	Joback Method

cpg	243.55	J/molxK	710.40	Joback Method
cpg	249.42	J/molxK	749.79	Joback Method
dvisc	0.0013398	Paxs	322.39	Joback Method
dvisc	0.0009161	Paxs	354.24	Joback Method
dvisc	0.0006669	Paxs	386.08	Joback Method
dvisc	0.0005096	Paxs	417.93	Joback Method
dvisc	0.0004045	Paxs	449.78	Joback Method
dvisc	0.0003311	Paxs	481.62	Joback Method
dvisc	0.0002778	Paxs	513.47	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	502.70	K	95.50	NIST Webbook

## Sources

<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=C6639301&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6639301&amp;Units=SI</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>

## 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>ie:</b>	Ionization energy
<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>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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