

# 1,1,2,2,3-pentachloropropane

<b>Inchi:</b>	InChI=1S/C3H3Cl5/c4-1-3(7,8)2(5)6/h2H,1H2
<b>InchiKey:</b>	IYFMQUDCYNWFTL-UHFFFAOYSA-N
<b>Formula:</b>	C3H3Cl5
<b>SMILES:</b>	C1CC(Cl)(Cl)C(Cl)Cl
<b>Mol. weight [g/mol]:</b>	216.32
<b>CAS:</b>	16714-68-4

## Physical Properties

Property code	Value	Unit	Source
gf	-84.87	kJ/mol	Joback Method
hf	-197.98	kJ/mol	Joback Method
hfus	13.57	kJ/mol	Joback Method
hvap	42.51	kJ/mol	Joback Method
log10ws	-3.06		Crippen Method
logp	3.203		Crippen Method
mcvol	114.330	ml/mol	McGowan Method
pc	3611.55	kPa	Joback Method
tb	451.52	K	Joback Method
tc	677.69	K	Joback Method
tf	260.59	K	Joback Method
vc	0.431	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	199.09	J/molxK	677.69	Joback Method
cpg	171.76	J/molxK	451.52	Joback Method
cpg	177.65	J/molxK	489.22	Joback Method
cpg	182.95	J/molxK	526.91	Joback Method
cpg	187.69	J/molxK	564.61	Joback Method
cpg	191.94	J/molxK	602.30	Joback Method
cpg	195.72	J/molxK	640.00	Joback Method
dvisc	0.0004208	Paxs	451.52	Joback Method
dvisc	0.0069460	Paxs	260.59	Joback Method

dvisc	0.0033757	Paxs	292.41	Joback Method
dvisc	0.0018901	Paxs	324.23	Joback Method
dvisc	0.0011739	Paxs	356.06	Joback Method
dvisc	0.0007884	Paxs	387.88	Joback Method
dvisc	0.0005624	Paxs	419.70	Joback Method
hvapt	46.30	kJ/mol	406.00	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=C16714684&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C16714684&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>hvapt:</b>	Enthalpy of vaporization at a given temperature
<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>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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