

# Heptane, 1,1,1-trichloro

<b>Inchi:</b>	InChI=1S/C7H13Cl3/c1-2-3-4-5-6-7(8,9)10/h2-6H2,1H3
<b>InchiKey:</b>	XQFUVDNFWZHPEJ-UHFFFAOYSA-N
<b>Formula:</b>	C7H13Cl3
<b>SMILES:</b>	CCCCCCC(Cl)(Cl)Cl
<b>Mol. weight [g/mol]:</b>	203.54

## Physical Properties

Property code	Value	Unit	Source
gf	-24.89	kJ/mol	Joback Method
hf	-243.78	kJ/mol	Joback Method
hfus	19.06	kJ/mol	Joback Method
hvap	43.03	kJ/mol	Joback Method
log10ws	-4.31		Crippen Method
logp	4.327		Crippen Method
mcvol	146.210	ml/mol	McGowan Method
pc	2545.61	kPa	Joback Method
rinpola	1151.00		NIST Webbook
rinpola	1151.00		NIST Webbook
tb	468.62	K	Joback Method
tc	665.55	K	Joback Method
tf	260.83	K	Joback Method
vc	0.564	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	280.69	J/molxK	468.62	Joback Method
cpg	333.52	J/molxK	632.73	Joback Method
cpg	324.25	J/molxK	599.91	Joback Method
cpg	314.36	J/molxK	567.08	Joback Method
cpg	303.83	J/molxK	534.26	Joback Method
cpg	292.62	J/molxK	501.44	Joback Method
cpg	342.23	J/molxK	665.55	Joback Method
dvisc	0.0003172	Paxs	468.62	Joback Method

dvisc	0.0004254	Paxs	433.99	Joback Method
dvisc	0.0006003	Paxs	399.36	Joback Method
dvisc	0.0009045	Paxs	364.73	Joback Method
dvisc	0.0014852	Paxs	330.09	Joback Method
dvisc	0.0027395	Paxs	295.46	Joback Method
dvisc	0.0059448	Paxs	260.83	Joback Method

## Sources

<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>
<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=R515365&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R515365&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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