

# 3-Chloropropyl heptanoate

<b>Other names:</b>	1-Propanol, 3-chloro, heptanoate
<b>Inchi:</b>	InChI=1S/C10H19ClO2/c1-2-3-4-5-7-10(12)13-9-6-8-11/h2-9H2,1H3
<b>InchiKey:</b>	PSGFDTBGMJYBCY-UHFFFAOYSA-N
<b>Formula:</b>	C10H19ClO2
<b>SMILES:</b>	CCCCCCC(=O)OCCCl
<b>Mol. weight [g/mol]:</b>	206.71

## Physical Properties

Property code	Value	Unit	Source
gf	-212.53	kJ/mol	Joback Method
hf	-510.27	kJ/mol	Joback Method
hfus	28.64	kJ/mol	Joback Method
hvap	51.39	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	3.129		Crippen Method
mvol	171.440	ml/mol	McGowan Method
pc	2125.60	kPa	Joback Method
rinpol	1413.00		NIST Webbook
rinpol	1413.00		NIST Webbook
tb	541.92	K	Joback Method
tc	719.34	K	Joback Method
tf	304.54	K	Joback Method
vc	0.668	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.46	J/molxK	541.92	Joback Method
cpg	461.13	J/molxK	689.77	Joback Method
cpg	449.68	J/molxK	660.20	Joback Method
cpg	437.70	J/molxK	630.63	Joback Method
cpg	425.18	J/molxK	601.06	Joback Method
cpg	412.10	J/molxK	571.49	Joback Method
cpg	472.05	J/molxK	719.34	Joback Method

dvisc	0.0002192	Paxs	541.92	Joback Method
dvisc	0.0002844	Paxs	502.36	Joback Method
dvisc	0.0003858	Paxs	462.79	Joback Method
dvisc	0.0005540	Paxs	423.23	Joback Method
dvisc	0.0008572	Paxs	383.67	Joback Method
dvisc	0.0014664	Paxs	344.10	Joback Method
dvisc	0.0028840	Paxs	304.54	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R34280&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R34280&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>
<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>

## 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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