

# Chloroacetic acid, heptyl ester

<b>Other names:</b>	Heptyl chloroacetate 1-Heptanol, chloroacetate
<b>Inchi:</b>	InChI=1S/C9H17ClO2/c1-2-3-4-5-6-7-12-9(11)8-10/h2-8H2,1H3
<b>InchiKey:</b>	JUFPTDUONWPUBM-UHFFFAOYSA-N
<b>Formula:</b>	C9H17ClO2
<b>SMILES:</b>	CCCCCCCOC(=O)CCI
<b>Mol. weight [g/mol]:</b>	192.68
<b>CAS:</b>	34589-22-5

## Physical Properties

Property code	Value	Unit	Source
gf	-220.95	kJ/mol	Joback Method
hf	-489.63	kJ/mol	Joback Method
hfus	26.05	kJ/mol	Joback Method
hvap	49.17	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	2.739		Crippen Method
mcvol	157.350	ml/mol	McGowan Method
pc	2327.03	kPa	Joback Method
rinpol	1305.00		NIST Webbook
rinpol	1296.00		NIST Webbook
rinpol	1275.00		NIST Webbook
rinpol	1276.00		NIST Webbook
rinpol	1293.00		NIST Webbook
rinpol	1297.00		NIST Webbook
rinpol	1307.00		NIST Webbook
rinpol	1319.00		NIST Webbook
ripol	1797.00		NIST Webbook
ripol	1788.00		NIST Webbook
ripol	1785.00		NIST Webbook
tb	519.04	K	Joback Method
tc	698.13	K	Joback Method
tf	293.27	K	Joback Method
vc	0.613	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.11	J/molxK	519.04	Joback Method
cpg	364.91	J/molxK	548.89	Joback Method
cpg	377.20	J/molxK	578.74	Joback Method
cpg	388.97	J/molxK	608.58	Joback Method
cpg	400.25	J/molxK	638.43	Joback Method
cpg	411.03	J/molxK	668.28	Joback Method
cpg	421.32	J/molxK	698.13	Joback Method
dvisc	0.0029830	Paxs	293.27	Joback Method
dvisc	0.0015445	Paxs	330.90	Joback Method
dvisc	0.0009148	Paxs	368.53	Joback Method
dvisc	0.0005970	Paxs	406.15	Joback Method
dvisc	0.0004189	Paxs	443.78	Joback Method
dvisc	0.0003106	Paxs	481.41	Joback Method
dvisc	0.0002406	Paxs	519.04	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=C34589225&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C34589225&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>ripol:</b>	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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