

# 5-Chlorovaleric acid, 4-hexadecyl ester

<b>Inchi:</b>	InChI=1S/C21H41ClO2/c1-3-5-6-7-8-9-10-11-12-13-17-20(16-4-2)24-21(23)18-14-15-19
<b>InchiKey:</b>	XTQZSUCQERUSLW-UHFFFAOYSA-N
<b>Formula:</b>	C21H41ClO2
<b>SMILES:</b>	CCCCCCCCCCCC(CCC)OC(=O)CCCCCI
<b>Mol. weight [g/mol]:</b>	361.00

## Physical Properties

Property code	Value	Unit	Source
gf	-122.35	kJ/mol	Joback Method
hf	-742.59	kJ/mol	Joback Method
hfus	53.61	kJ/mol	Joback Method
hvap	75.49	kJ/mol	Joback Method
log10ws	-7.74		Crippen Method
logp	7.418		Crippen Method
mvol	326.430	ml/mol	McGowan Method
pc	966.27	kPa	Joback Method
rinpol	2393.40		NIST Webbook
rinpol	2393.40		NIST Webbook
tb	793.16	K	Joback Method
tc	974.19	K	Joback Method
tf	413.51	K	Joback Method
vc	1.278	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1005.53	J/molxK	793.16	Joback Method
cpg	1024.93	J/molxK	823.33	Joback Method
cpg	1043.31	J/molxK	853.50	Joback Method
cpg	1060.71	J/molxK	883.67	Joback Method
cpg	1077.14	J/molxK	913.85	Joback Method
cpg	1092.65	J/molxK	944.02	Joback Method
cpg	1107.26	J/molxK	974.19	Joback Method
dvisc	0.0014045	Paxs	413.51	Joback Method

dvisc	0.0005600	Paxs	476.78	Joback Method
dvisc	0.0002769	Paxs	540.06	Joback Method
dvisc	0.0001588	Paxs	603.34	Joback Method
dvisc	0.0001012	Paxs	666.61	Joback Method
dvisc	0.0000697	Paxs	729.88	Joback Method
dvisc	0.0000509	Paxs	793.16	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U292248&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U292248&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>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</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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