

# 5-Chlorovaleric acid, cyclobutyl ester

Inchi:	InChI=1S/C9H15ClO2/c10-7-2-1-6-9(11)12-8-4-3-5-8/h8H,1-7H2
InchiKey:	IJPXXYJIZRATCH-UHFFFAOYSA-N
Formula:	C9H15ClO2
SMILES:	O=C(CCCCCI)OC1CCC1
Mol. weight [g/mol]:	190.67

## Physical Properties

Property code	Value	Unit	Source
gf	-172.30	kJ/mol	Joback Method
hf	-422.99	kJ/mol	Joback Method
hfus	22.09	kJ/mol	Joback Method
hvap	49.25	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	2.491		Crippen Method
mvol	146.490	ml/mol	McGowan Method
pc	2718.33	kPa	Joback Method
rinpol	1389.30		NIST Webbook
tb	530.05	K	Joback Method
tc	728.93	K	Joback Method
tf	307.69	K	Joback Method
vc	0.561	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	337.92	J/molxK	530.05	Joback Method
cpg	402.70	J/molxK	695.78	Joback Method
cpg	391.16	J/molxK	662.63	Joback Method
cpg	378.93	J/molxK	629.49	Joback Method
cpg	366.00	J/molxK	596.34	Joback Method
cpg	352.34	J/molxK	563.20	Joback Method
cpg	413.59	J/molxK	728.93	Joback Method
dvisc	0.0004062	Paxs	530.05	Joback Method
dvisc	0.0004951	Paxs	492.99	Joback Method

dvisc	0.0006231	Paxs	455.93	Joback Method
dvisc	0.0008169	Paxs	418.87	Joback Method
dvisc	0.0011286	Paxs	381.81	Joback Method
dvisc	0.0016715	Paxs	344.75	Joback Method
dvisc	0.0027213	Paxs	307.69	Joback Method

## Sources

<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=U292241&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U292241&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>

## 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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