

# 4-Chlorobutyric acid, 8-chlorooctyl ester

Inchi:	InChI=1S/C12H22Cl2O2/c13-9-5-3-1-2-4-6-11-16-12(15)8-7-10-14/h1-11H2
InchiKey:	IGLCKPGKGGWWLBI-UHFFFAOYSA-N
Formula:	C12H22Cl2O2
SMILES:	O=C(CCCCl)OCCCCCCCCCl
Mol. weight [g/mol]:	269.21

## Physical Properties

Property code	Value	Unit	Source
gf	-207.62	kJ/mol	Joback Method
hf	-567.29	kJ/mol	Joback Method
hfus	38.02	kJ/mol	Joback Method
hvap	60.23	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	4.128		Crippen Method
mvol	211.860	ml/mol	McGowan Method
pc	1739.01	kPa	Joback Method
rinpol	1963.00		NIST Webbook
rinpol	1963.00		NIST Webbook
tb	625.11	K	Joback Method
tc	804.22	K	Joback Method
tf	357.00	K	Joback Method
vc	0.830	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.01	J/molxK	625.11	Joback Method
cpg	541.35	J/molxK	654.96	Joback Method
cpg	555.02	J/molxK	684.81	Joback Method
cpg	568.05	J/molxK	714.67	Joback Method
cpg	580.44	J/molxK	744.52	Joback Method
cpg	592.21	J/molxK	774.37	Joback Method
cpg	603.37	J/molxK	804.22	Joback Method
dvisc	0.0021690	Paxs	357.00	Joback Method

dvisc	0.0011095	Paxs	401.69	Joback Method
dvisc	0.0006490	Paxs	446.37	Joback Method
dvisc	0.0004186	Paxs	491.05	Joback Method
dvisc	0.0002905	Paxs	535.74	Joback Method
dvisc	0.0002132	Paxs	580.42	Joback Method
dvisc	0.0001636	Paxs	625.11	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=U360644&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U360644&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>cp<sub>g</sub>:</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>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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