

# Chloromethyl 10-chlorododecanoate

<b>Other names:</b>	10-Chlorododecanoic acid, chloromethyl ester
<b>Inchi:</b>	InChI=1S/C13H24Cl2O2/c1-2-12(15)9-7-5-3-4-6-8-10-13(16)17-11-14/h12H,2-11H2,1H3
<b>InchiKey:</b>	CKRGKKRODIRREL-UHFFFAOYSA-N
<b>Formula:</b>	C13H24Cl2O2
<b>SMILES:</b>	CCC(Cl)CCCCCCCCC(=O)OCCI
<b>Mol. weight [g/mol]:</b>	283.23
<b>CAS:</b>	80419-06-3

## Physical Properties

Property code	Value	Unit	Source
gf	-201.64	kJ/mol	Joback Method
hf	-593.21	kJ/mol	Joback Method
hfus	37.08	kJ/mol	Joback Method
hvap	62.07	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	4.864		Crippen Method
mcvol	225.950	ml/mol	McGowan Method
pc	1618.07	kPa	Joback Method
rinpol	1940.00		NIST Webbook
rinpol	1905.00		NIST Webbook
rinpol	1910.00		NIST Webbook
rinpol	1895.00		NIST Webbook
rinpol	1895.00		NIST Webbook
ripol	2512.00		NIST Webbook
ripol	2480.00		NIST Webbook
ripol	2506.00		NIST Webbook
ripol	2480.00		NIST Webbook
tb	647.55	K	Joback Method
tc	828.32	K	Joback Method
tf	353.27	K	Joback Method
vc	0.879	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	579.55	J/mol×K	647.55	Joback Method
cpg	594.71	J/mol×K	677.68	Joback Method
cpg	609.14	J/mol×K	707.81	Joback Method
cpg	622.86	J/mol×K	737.94	Joback Method
cpg	635.88	J/mol×K	768.06	Joback Method
cpg	648.22	J/mol×K	798.19	Joback Method
cpg	659.91	J/mol×K	828.32	Joback Method
dvisc	0.0025326	Paxs	353.27	Joback Method
dvisc	0.0011518	Paxs	402.32	Joback Method
dvisc	0.0006217	Paxs	451.36	Joback Method
dvisc	0.0003786	Paxs	500.41	Joback Method
dvisc	0.0002520	Paxs	549.46	Joback Method
dvisc	0.0001792	Paxs	598.50	Joback Method
dvisc	0.0001343	Paxs	647.55	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=C80419063&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C80419063&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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</b>	Non-polar retention indices
<b>ripola:</b>	Polar retention indices

**tb:** Normal Boiling Point Temperature  
**tc:** Critical Temperature  
**tf:** Normal melting (fusion) point  
**vc:** Critical Volume

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