

# 4-Chlorobenzoic acid, undecyl ester

<b>Other names:</b>	Undecyl 4-chlorobenzoate
<b>Inchi:</b>	InChI=1S/C18H27ClO2/c1-2-3-4-5-6-7-8-9-10-15-21-18(20)16-11-13-17(19)14-12-16/h1
<b>InchiKey:</b>	MEWVVEWZGJOCOB-UHFFFAOYSA-N
<b>Formula:</b>	C18H27ClO2
<b>SMILES:</b>	CCCCCCCCCCCCOC(=O)c1ccc(Cl)cc1
<b>Mol. weight [g/mol]:</b>	310.86
<b>CAS:</b>	5458-41-3

## Physical Properties

Property code	Value	Unit	Source
gf	-42.39	kJ/mol	Joback Method
hf	-450.33	kJ/mol	Joback Method
hfus	43.01	kJ/mol	Joback Method
hvap	72.14	kJ/mol	Joback Method
log10ws	-6.58		Crippen Method
logp	6.028		Crippen Method
mcvol	260.400	ml/mol	McGowan Method
pc	1455.68	kPa	Joback Method
rinpol	2212.00		NIST Webbook
tb	756.62	K	Joback Method
tc	953.54	K	Joback Method
tf	433.64	K	Joback Method
vc	1.008	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	741.39	J/mol×K	756.62	Joback Method
cpg	814.71	J/mol×K	920.72	Joback Method
cpg	801.89	J/mol×K	887.90	Joback Method
cpg	788.18	J/mol×K	855.08	Joback Method
cpg	773.55	J/mol×K	822.26	Joback Method
cpg	757.96	J/mol×K	789.44	Joback Method
cpg	826.67	J/mol×K	953.54	Joback Method

dvisc	0.0000856	Paxs	756.62	Joback Method
dvisc	0.0001106	Paxs	702.79	Joback Method
dvisc	0.0001490	Paxs	648.96	Joback Method
dvisc	0.0002119	Paxs	595.13	Joback Method
dvisc	0.0003232	Paxs	541.30	Joback Method
dvisc	0.0005413	Paxs	487.47	Joback Method
dvisc	0.0010302	Paxs	433.64	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=C5458413&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5458413&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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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