

# 4-Chlorobenzoic acid, undec-2-enyl ester

<b>Inchi:</b>	InChI=1S/C18H25ClO2/c1-2-3-4-5-6-7-8-9-10-15-21-18(20)16-11-13-17(19)14-12-16/h9-
<b>InchiKey:</b>	OECIAGVCGLDHIB-MDZDMXLPSA-N
<b>Formula:</b>	C18H25ClO2
<b>SMILES:</b>	CCCCCCCC=CCOC(=O)c1ccc(Cl)cc1
<b>Mol. weight [g/mol]:</b>	308.84

## Physical Properties

Property code	Value	Unit	Source
gf	37.83	kJ/mol	Joback Method
hf	-333.11	kJ/mol	Joback Method
hfus	43.21	kJ/mol	Joback Method
hvap	72.10	kJ/mol	Joback Method
log10ws	-6.44		Crippen Method
logp	5.804		Crippen Method
mvol	256.100	ml/mol	McGowan Method
pc	1515.21	kPa	Joback Method
rmpol	2241.00		NIST Webbook
tb	760.78	K	Joback Method
tc	963.40	K	Joback Method
tf	428.56	K	Joback Method
vc	0.989	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	716.95	J/molxK	760.78	Joback Method
cpg	733.04	J/molxK	794.55	Joback Method
cpg	748.15	J/molxK	828.32	Joback Method
cpg	762.34	J/molxK	862.09	Joback Method
cpg	775.65	J/molxK	895.86	Joback Method
cpg	788.12	J/molxK	929.63	Joback Method
cpg	799.79	J/molxK	963.40	Joback Method
dvisc	0.0009520	Paxs	428.56	Joback Method
dvisc	0.0004880	Paxs	483.93	Joback Method

dvisc	0.0002869	Paxs	539.30	Joback Method
dvisc	0.0001862	Paxs	594.67	Joback Method
dvisc	0.0001301	Paxs	650.04	Joback Method
dvisc	0.0000962	Paxs	705.41	Joback Method
dvisc	0.0000743	Paxs	760.78	Joback Method

## Sources

<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=U299370&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299370&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>

## 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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