

# 2-Chlorobenzoic acid, 5-tetradecyl ester

<b>Inchi:</b>	InChI=1S/C21H33ClO2/c1-3-5-7-8-9-10-11-15-18(14-6-4-2)24-21(23)19-16-12-13-17-20
<b>InchiKey:</b>	HBSHCUYTTUNVEU-UHFFFAOYSA-N
<b>Formula:</b>	C21H33ClO2
<b>SMILES:</b>	CCCCCCCCC(CCCC)OC(=O)c1ccccc1Cl
<b>Mol. weight [g/mol]:</b>	352.94

## Physical Properties

Property code	Value	Unit	Source
gf	-19.57	kJ/mol	Joback Method
hf	-517.53	kJ/mol	Joback Method
hfus	47.26	kJ/mol	Joback Method
hvap	78.43	kJ/mol	Joback Method
log10ws	-7.95		Crippen Method
logp	7.196		Crippen Method
mvol	302.670	ml/mol	McGowan Method
pc	1188.24	kPa	Joback Method
rinpol	2376.00		NIST Webbook
tb	824.82	K	Joback Method
tc	1023.18	K	Joback Method
tf	452.45	K	Joback Method
vc	1.171	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	916.82	J/molxK	824.82	Joback Method
cpg	993.70	J/molxK	990.12	Joback Method
cpg	980.36	J/molxK	957.06	Joback Method
cpg	966.05	J/molxK	924.00	Joback Method
cpg	950.71	J/molxK	890.94	Joback Method
cpg	934.32	J/molxK	857.88	Joback Method
cpg	1006.09	J/molxK	1023.18	Joback Method
dvisc	0.0000523	Paxs	824.82	Joback Method
dvisc	0.0000693	Paxs	762.76	Joback Method

dvisc	0.0000965	Paxs	700.70	Joback Method
dvisc	0.0001432	Paxs	638.63	Joback Method
dvisc	0.0002314	Paxs	576.57	Joback Method
dvisc	0.0004199	Paxs	514.51	Joback Method
dvisc	0.0008970	Paxs	452.45	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=U299820&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299820&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>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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