

# 2-Chlorobenzoic acid, 6-pentadecyl ester

<b>Inchi:</b>	InChI=1S/C22H35ClO2/c1-3-5-7-8-9-10-12-16-19(15-11-6-4-2)25-22(24)20-17-13-14-18
<b>InchiKey:</b>	LAECTIQLWWUWOK-UHFFFAOYSA-N
<b>Formula:</b>	C22H35ClO2
<b>SMILES:</b>	CCCCCCCCC(CCCCC)OC(=O)c1ccccc1Cl
<b>Mol. weight [g/mol]:</b>	366.96

## Physical Properties

Property code	Value	Unit	Source
gf	-11.15	kJ/mol	Joback Method
hf	-538.17	kJ/mol	Joback Method
hfus	49.85	kJ/mol	Joback Method
hvap	80.66	kJ/mol	Joback Method
log10ws	-8.37		Crippen Method
logp	7.586		Crippen Method
mcvol	316.760	ml/mol	McGowan Method
pc	1113.34	kPa	Joback Method
rinpola	2464.00		NIST Webbook
tb	847.70	K	Joback Method
tc	1046.95	K	Joback Method
tf	463.72	K	Joback Method
vc	1.226	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	976.83	J/molxK	847.70	Joback Method
cpg	994.55	J/molxK	880.91	Joback Method
cpg	1011.14	J/molxK	914.12	Joback Method
cpg	1026.64	J/molxK	947.33	Joback Method
cpg	1041.09	J/molxK	980.54	Joback Method
cpg	1054.54	J/molxK	1013.74	Joback Method
cpg	1067.03	J/molxK	1046.95	Joback Method
dvisc	0.0008036	Paxs	463.72	Joback Method
dvisc	0.0003724	Paxs	527.72	Joback Method

dvisc	0.0002038	Paxs	591.71	Joback Method
dvisc	0.0001254	Paxs	655.71	Joback Method
dvisc	0.0000842	Paxs	719.71	Joback Method
dvisc	0.0000603	Paxs	783.70	Joback Method
dvisc	0.0000454	Paxs	847.70	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=U299825&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299825&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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