

# 4-Chlorobenzoic acid, 2-pentyl ester

Other names:	Benzoic acid, 4-chloro, 1-methylbutyl ester
Inchi:	InChI=1S/C12H15ClO2/c1-3-4-9(2)15-12(14)10-5-7-11(13)8-6-10/h5-9H,3-4H2,1-2H3
InchiKey:	YAOLJHAAVJEVSU-UHFFFAOYSA-N
Formula:	C12H15ClO2
SMILES:	CCCC(C)OC(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]:	226.70
CAS:	97989-39-4

## Physical Properties

Property code	Value	Unit	Source
gf	-95.35	kJ/mol	Joback Method
hf	-331.77	kJ/mol	Joback Method
hfus	23.95	kJ/mol	Joback Method
hvap	58.40	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.685		Crippen Method
mcvol	175.860	ml/mol	McGowan Method
pc	2410.00	kPa	Joback Method
rinpol	1533.00		NIST Webbook
rinpol	1550.00		NIST Webbook
rinpol	1551.00		NIST Webbook
rinpol	1532.00		NIST Webbook
rinpol	1540.00		NIST Webbook
rinpol	1542.00		NIST Webbook
ripol	2036.00		NIST Webbook
ripol	2054.00		NIST Webbook
ripol	2020.00		NIST Webbook
ripol	2041.00		NIST Webbook
ripol	2019.00		NIST Webbook
ripol	2054.00		NIST Webbook
ripol	2054.00		NIST Webbook
ripol	2019.00		NIST Webbook
tb	618.90	K	Joback Method
tc	834.03	K	Joback Method
tf	351.02	K	Joback Method
vc	0.666	m3/kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.78	J/molxK	618.90	Joback Method
cpg	436.13	J/molxK	654.76	Joback Method
cpg	449.61	J/molxK	690.61	Joback Method
cpg	462.25	J/molxK	726.47	Joback Method
cpg	474.07	J/molxK	762.32	Joback Method
cpg	485.09	J/molxK	798.18	Joback Method
cpg	495.33	J/molxK	834.03	Joback Method
dvisc	0.0019039	Paxs	351.02	Joback Method
dvisc	0.0010010	Paxs	395.67	Joback Method
dvisc	0.0005996	Paxs	440.31	Joback Method
dvisc	0.0003947	Paxs	484.96	Joback Method
dvisc	0.0002788	Paxs	529.61	Joback Method
dvisc	0.0002079	Paxs	574.25	Joback Method
dvisc	0.0001617	Paxs	618.90	Joback Method

## Sources

Joback Method:	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C97989394&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C97989394&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>ripol:</b>	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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