

# 4-Chlorobutyl benzoate

<b>Inchi:</b>	InChI=1S/C11H13ClO2/c12-8-4-5-9-14-11(13)10-6-2-1-3-7-10/h1-3,6-7H,4-5,8-9H2
<b>InchiKey:</b>	XFFQVVCNZAYQSJ-UHFFFAOYSA-N
<b>Formula:</b>	C11H13ClO2
<b>SMILES:</b>	O=C(OCCCCl)c1ccccc1
<b>Mol. weight [g/mol]:</b>	212.67
<b>CAS:</b>	946-02-1

## Physical Properties

Property code	Value	Unit	Source
gf	-91.70	kJ/mol	Joback Method
hf	-294.38	kJ/mol	Joback Method
hfus	25.27	kJ/mol	Joback Method
hvap	55.90	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	2.862		Crippen Method
mcvol	161.770	ml/mol	McGowan Method
pc	2673.54	kPa	Joback Method
tb	591.48	K	Joback Method
tc	804.91	K	Joback Method
tf	342.23	K	Joback Method
vc	0.617	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.49	J/molxK	591.48	Joback Method
cpg	387.05	J/molxK	627.05	Joback Method
cpg	399.78	J/molxK	662.62	Joback Method
cpg	411.71	J/molxK	698.20	Joback Method
cpg	422.86	J/molxK	733.77	Joback Method
cpg	433.26	J/molxK	769.34	Joback Method
cpg	442.93	J/molxK	804.91	Joback Method
dvisc	0.0020741	Paxs	342.23	Joback Method
dvisc	0.0011303	Paxs	383.77	Joback Method

dvisc	0.0006935	Paxs	425.31	Joback Method
dvisc	0.0004642	Paxs	466.86	Joback Method
dvisc	0.0003317	Paxs	508.40	Joback Method
dvisc	0.0002494	Paxs	549.94	Joback Method
dvisc	0.0001952	Paxs	591.48	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	414.50 ± 1.50	K	0.70	NIST Webbook

## 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=C946021&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C946021&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>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point

**vc:** Critical Volume

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