

# Benzoic acid, 4-chloro-, butyl ester

<b>Other names:</b>	4-Chlorobenzoic acid, butyl ester Butyl 4-chlorobenzoate
<b>Inchi:</b>	InChI=1S/C11H13ClO2/c1-2-3-8-14-11(13)9-4-6-10(12)7-5-9/h4-7H,2-3,8H2,1H3
<b>InchiKey:</b>	PBPVJPWUWLGOEC-UHFFFAOYSA-N
<b>Formula:</b>	C11H13ClO2
<b>SMILES:</b>	CCCCOC(=O)c1ccc(Cl)cc1
<b>Mol. weight [g/mol]:</b>	212.67
<b>CAS:</b>	27942-64-9

## Physical Properties

Property code	Value	Unit	Source
gf	-101.33	kJ/mol	Joback Method
hf	-305.85	kJ/mol	Joback Method
hfus	24.88	kJ/mol	Joback Method
hvap	56.56	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	3.297		Crippen Method
mcvol	161.770	ml/mol	McGowan Method
pc	2632.55	kPa	Joback Method
rinpol	1518.00		NIST Webbook
rinpol	1539.00		NIST Webbook
rinpol	1524.00		NIST Webbook
rinpol	1508.00		NIST Webbook
rinpol	1518.00		NIST Webbook
rinpol	1518.00		NIST Webbook
rinpol	1528.00		NIST Webbook
rinpol	1524.00		NIST Webbook
ripol	2038.00		NIST Webbook
ripol	2102.00		NIST Webbook
ripol	2057.00		NIST Webbook
ripol	2065.00		NIST Webbook
ripol	2073.00		NIST Webbook
ripol	2017.00		NIST Webbook
tb	596.46	K	Joback Method
tc	810.87	K	Joback Method
tf	354.75	K	Joback Method
vc	0.617	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.82	J/molxK	596.46	Joback Method
cpg	386.14	J/molxK	632.19	Joback Method
cpg	398.67	J/molxK	667.93	Joback Method
cpg	410.44	J/molxK	703.66	Joback Method
cpg	421.46	J/molxK	739.40	Joback Method
cpg	431.76	J/molxK	775.13	Joback Method
cpg	441.35	J/molxK	810.87	Joback Method
dvisc	0.0016178	Paxs	354.75	Joback Method
dvisc	0.0009457	Paxs	395.04	Joback Method
dvisc	0.0006105	Paxs	435.32	Joback Method
dvisc	0.0004245	Paxs	475.61	Joback Method
dvisc	0.0003124	Paxs	515.89	Joback Method
dvisc	0.0002403	Paxs	556.17	Joback Method
dvisc	0.0001915	Paxs	596.46	Joback Method

## Sources

<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=C27942649&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C27942649&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>
<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>

## 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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