

# Benzoyl chloride, 4-butyl-

<b>Other names:</b>	4-Butylbenzoyl chloride p-Butylbenzoyl chloride 4-n-Butylbenzoyl chloride
<b>Inchi:</b>	InChI=1S/C11H13ClO/c1-2-3-4-9-5-7-10(8-6-9)11(12)13/h5-8H,2-4H2,1H3
<b>InchiKey:</b>	OUOWCSJYDCPVDM-UHFFFAOYSA-N
<b>Formula:</b>	C11H13ClO
<b>SMILES:</b>	CCCCc1ccc(C(=O)Cl)cc1
<b>Mol. weight [g/mol]:</b>	196.67
<b>CAS:</b>	28788-62-7

## Physical Properties

Property code	Value	Unit	Source
gf	3.67	kJ/mol	Joback Method
hf	-173.63	kJ/mol	Joback Method
hfus	23.69	kJ/mol	Joback Method
hvap	54.15	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	3.408		Crippen Method
mcvol	155.900	ml/mol	McGowan Method
pc	2679.08	kPa	Joback Method
rinpol	1522.00		NIST Webbook
tb	574.04	K	Joback Method
tc	790.99	K	Joback Method
tf	332.52	K	Joback Method
vc	0.599	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.64	J/molxK	574.04	Joback Method
cpg	362.22	J/molxK	610.20	Joback Method
cpg	374.97	J/molxK	646.36	Joback Method
cpg	386.91	J/molxK	682.52	Joback Method
cpg	398.09	J/molxK	718.67	Joback Method

cpg	408.53	J/molxK	754.83	Joback Method
cpg	418.27	J/molxK	790.99	Joback Method
dvisc	0.0021679	Paxs	332.52	Joback Method
dvisc	0.0012297	Paxs	372.77	Joback Method
dvisc	0.0007791	Paxs	413.03	Joback Method
dvisc	0.0005352	Paxs	453.28	Joback Method
dvisc	0.0003909	Paxs	493.53	Joback Method
dvisc	0.0002994	Paxs	533.79	Joback Method
dvisc	0.0002380	Paxs	574.04	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	428.70	K	2.90	NIST Webbook

## Sources

<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=C28788627&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C28788627&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>

## 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>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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