

# Butanoic acid, 4-chlorophenyl ester

<b>Other names:</b>	Butyric acid, p-chlorophenyl ester 4-Chlorophenyl butyrate Butyric acid, 4-chlorophenyl ester p-Chlorophenyl butyrate
<b>Inchi:</b>	InChI=1S/C10H11ClO2/c1-2-3-10(12)13-9-6-4-8(11)5-7-9/h4-7H,2-3H2,1H3
<b>InchiKey:</b>	CLXDRKZHOMSWBH-UHFFFAOYSA-N
<b>Formula:</b>	C10H11ClO2
<b>SMILES:</b>	CCCC(=O)Oc1ccc(Cl)cc1
<b>Mol. weight [g/mol]:</b>	198.65
<b>CAS:</b>	7476-81-5

## Physical Properties

Property code	Value	Unit	Source
gf	-109.75	kJ/mol	Joback Method
hf	-285.21	kJ/mol	Joback Method
hfus	22.29	kJ/mol	Joback Method
hvap	54.33	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	3.046		Crippen Method
mcvol	147.680	ml/mol	McGowan Method
pc	2912.39	kPa	Joback Method
rinpol	1393.00		NIST Webbook
rinpol	1393.00		NIST Webbook
tb	573.58	K	Joback Method
tc	791.74	K	Joback Method
tf	343.48	K	Joback Method
vc	0.560	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.95	J/mol×K	573.58	Joback Method
cpg	381.22	J/mol×K	755.38	Joback Method
cpg	371.57	J/mol×K	719.02	Joback Method

cpg	361.23	J/molxK	682.66	Joback Method
cpg	350.20	J/molxK	646.30	Joback Method
cpg	338.44	J/molxK	609.94	Joback Method
cpg	390.20	J/molxK	791.74	Joback Method
dvisc	0.0002099	Paxs	573.58	Joback Method
dvisc	0.0002619	Paxs	535.23	Joback Method
dvisc	0.0003383	Paxs	496.88	Joback Method
dvisc	0.0004560	Paxs	458.53	Joback Method
dvisc	0.0006491	Paxs	420.18	Joback Method
dvisc	0.0009919	Paxs	381.83	Joback Method
dvisc	0.0016661	Paxs	343.48	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=C7476815&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C7476815&amp;Units=SI</a>
<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>

## 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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