

# 4-Chlorobenzoic acid, 2-methylpropyl ester

<b>Other names:</b>	Isobutyl 4-chlorobenzoate Benzoic acid, 4-chloro, isobutyl ester
<b>Inchi:</b>	InChI=1S/C11H13ClO2/c1-8(2)7-14-11(13)9-3-5-10(12)6-4-9/h3-6,8H,7H2,1-2H3
<b>InchiKey:</b>	BWLDEQAGSZRTIV-UHFFFAOYSA-N
<b>Formula:</b>	C11H13ClO2
<b>SMILES:</b>	CC(C)COC(=O)c1ccc(Cl)cc1
<b>Mol. weight [g/mol]:</b>	212.67
<b>CAS:</b>	29234-88-6

## Physical Properties

Property code	Value	Unit	Source
gf	-103.77	kJ/mol	Joback Method
hf	-311.13	kJ/mol	Joback Method
hfus	21.36	kJ/mol	Joback Method
hvap	56.17	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	3.153		Crippen Method
mcvol	161.770	ml/mol	McGowan Method
pc	2654.29	kPa	Joback Method
rinpol	1467.00		NIST Webbook
rinpol	1477.00		NIST Webbook
rinpol	1489.00		NIST Webbook
rinpol	1480.00		NIST Webbook
rinpol	1463.00		NIST Webbook
rinpol	1473.00		NIST Webbook
rinpol	1480.00		NIST Webbook
rinpol	1467.00		NIST Webbook
ripol	1994.00		NIST Webbook
ripol	1975.00		NIST Webbook
ripol	2009.00		NIST Webbook
ripol	1973.00		NIST Webbook
ripol	2012.00		NIST Webbook
ripol	1994.00		NIST Webbook
tb	596.02	K	Joback Method
tc	814.94	K	Joback Method
tf	339.75	K	Joback Method
vc	0.611	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.26	J/molxK	596.02	Joback Method
cpg	386.90	J/molxK	632.51	Joback Method
cpg	399.73	J/molxK	668.99	Joback Method
cpg	411.74	J/molxK	705.48	Joback Method
cpg	422.97	J/molxK	741.97	Joback Method
cpg	433.43	J/molxK	778.45	Joback Method
cpg	443.15	J/molxK	814.94	Joback Method
dvisc	0.0019955	Paxs	339.75	Joback Method
dvisc	0.0010666	Paxs	382.46	Joback Method
dvisc	0.0006465	Paxs	425.17	Joback Method
dvisc	0.0004294	Paxs	467.88	Joback Method
dvisc	0.0003054	Paxs	510.60	Joback Method
dvisc	0.0002290	Paxs	553.31	Joback Method
dvisc	0.0001789	Paxs	596.02	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=C29234886&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C29234886&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>ripol:</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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