

# 4-Chlorobutyric acid, 3,5-dimethylphenyl ester

<b>Inchi:</b>	InChI=1S/C12H15ClO2/c1-9-6-10(2)8-11(7-9)15-12(14)4-3-5-13/h6-8H,3-5H2,1-2H3
<b>InchiKey:</b>	BWWVMEDTGZFRCA-UHFFFAOYSA-N
<b>Formula:</b>	C12H15ClO2
<b>SMILES:</b>	Cc1cc(C)cc(OC(=O)CCCCl)c1
<b>Mol. weight [g/mol]:</b>	226.70

## Physical Properties

Property code	Value	Unit	Source
gf	-102.54	kJ/mol	Joback Method
hf	-337.96	kJ/mol	Joback Method
hfus	27.08	kJ/mol	Joback Method
hvap	59.45	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	3.228		Crippen Method
mcvol	175.860	ml/mol	McGowan Method
pc	2356.49	kPa	Joback Method
rinpol	1670.00		NIST Webbook
rinpol	1744.00		NIST Webbook
rinpol	1744.00		NIST Webbook
rinpol	1670.00		NIST Webbook
tb	624.32	K	Joback Method
tc	836.12	K	Joback Method
tf	378.54	K	Joback Method
vc	0.672	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.60	J/molxK	624.32	Joback Method
cpg	434.41	J/molxK	659.62	Joback Method
cpg	447.44	J/molxK	694.92	Joback Method
cpg	459.71	J/molxK	730.22	Joback Method
cpg	471.22	J/molxK	765.52	Joback Method
cpg	481.99	J/molxK	800.82	Joback Method

cpg	492.04	J/mol×K	836.12	Joback Method
dvisc	0.0012490	Paxs	378.54	Joback Method
dvisc	0.0007630	Paxs	419.50	Joback Method
dvisc	0.0005088	Paxs	460.47	Joback Method
dvisc	0.0003625	Paxs	501.43	Joback Method
dvisc	0.0002718	Paxs	542.39	Joback Method
dvisc	0.0002123	Paxs	583.36	Joback Method
dvisc	0.0001712	Paxs	624.32	Joback Method

## Sources

<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=U357772&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U357772&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>

## 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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