

# 1,2-Cyclohexanedicarboxylic acid, butyl 2-chlorophenyl ester

<b>Inchi:</b>	InChI=1S/C18H23ClO4/c1-2-3-12-22-17(20)13-8-4-5-9-14(13)18(21)23-16-11-7-6-10-15
<b>InchiKey:</b>	JDXKIHODWWBARN-UHFFFAOYSA-N
<b>Formula:</b>	C18H23ClO4
<b>SMILES:</b>	CCCCOC(=O)C1CCCCC1C(=O)Oc1ccccc1Cl
<b>Mol. weight [g/mol]:</b>	338.83

## Physical Properties

Property code	Value	Unit	Source
gf	-259.57	kJ/mol	Joback Method
hf	-661.15	kJ/mol	Joback Method
hfus	38.70	kJ/mol	Joback Method
hvap	81.42	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.395		Crippen Method
mcvol	256.980	ml/mol	McGowan Method
pc	1731.78	kPa	Joback Method
tb	847.79	K	Joback Method
tc	1074.08	K	Joback Method
tf	508.94	K	Joback Method
vc	0.965	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	786.53	J/molxK	847.79	Joback Method
cpg	851.03	J/molxK	1036.37	Joback Method
cpg	841.06	J/molxK	998.65	Joback Method
cpg	829.65	J/molxK	960.94	Joback Method
cpg	816.77	J/molxK	923.22	Joback Method
cpg	802.40	J/molxK	885.51	Joback Method
cpg	859.58	J/molxK	1074.08	Joback Method
dvisc	0.0000842	Paxs	847.79	Joback Method
dvisc	0.0001063	Paxs	791.32	Joback Method
dvisc	0.0001391	Paxs	734.84	Joback Method

dvisc	0.0001904	Paxs	678.37	Joback Method
dvisc	0.0002760	Paxs	621.89	Joback Method
dvisc	0.0004307	Paxs	565.41	Joback Method
dvisc	0.0007421	Paxs	508.94	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=U339584&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U339584&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307i">http://pubs.acs.org/doi/abs/10.1021/ci990307i</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>hvac:</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>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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