

# cis-Cyclohex-4-en-1,2-dicarboxylic acid, butyl 4-chloro-3-methylphenyl ester

<b>Inchi:</b>	InChI=1S/C19H23ClO4/c1-3-4-11-23-18(21)15-7-5-6-8-16(15)19(22)24-14-9-10-17(20)1
<b>InchiKey:</b>	XPGLRAPDLPZHLH-UHFFFAOYSA-N
<b>Formula:</b>	C19H23ClO4
<b>SMILES:</b>	CCCCOC(=O)C1CC=CCC1C(=O)Oc1ccc(Cl)c(C)c1
<b>Mol. weight [g/mol]:</b>	350.84

## Physical Properties

Property code	Value	Unit	Source
gf	-230.82	kJ/mol	Joback Method
hf	-635.48	kJ/mol	Joback Method
hfus	42.13	kJ/mol	Joback Method
hvap	84.60	kJ/mol	Joback Method
log10ws	-5.26		Crippen Method
logp	4.480		Crippen Method
mcvol	266.770	ml/mol	McGowan Method
pc	1628.54	kPa	Joback Method
tb	874.81	K	Joback Method
tc	1101.02	K	Joback Method
tf	533.49	K	Joback Method
vc	1.006	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	814.82	J/molxK	874.81	Joback Method
cpg	829.75	J/molxK	912.51	Joback Method
cpg	843.19	J/molxK	950.21	Joback Method
cpg	855.16	J/molxK	987.91	Joback Method
cpg	865.68	J/molxK	1025.62	Joback Method
cpg	874.77	J/molxK	1063.32	Joback Method
cpg	882.45	J/molxK	1101.02	Joback Method
dvisc	0.0005909	Paxs	533.49	Joback Method
dvisc	0.0003616	Paxs	590.38	Joback Method
dvisc	0.0002412	Paxs	647.26	Joback Method

dvisc	0.0001718	Paxs	704.15	Joback Method
dvisc	0.0001287	Paxs	761.04	Joback Method
dvisc	0.0001004	Paxs	817.92	Joback Method
dvisc	0.0000809	Paxs	874.81	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=U382648&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382648&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>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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