

# Isophthalic acid, butyl 4-chloro-3-methylphenyl ester

<b>Inchi:</b>	InChI=1S/C19H19ClO4/c1-3-4-10-23-18(21)14-6-5-7-15(12-14)19(22)24-16-8-9-17(20)1
<b>InchiKey:</b>	HMHLDFWHSIGOHI-UHFFFAOYSA-N
<b>Formula:</b>	C19H19ClO4
<b>SMILES:</b>	CCCCOC(=O)c1cccc(C(=O)Oc2ccc(Cl)c(C)c2)c1
<b>Mol. weight [g/mol]:</b>	346.81

## Physical Properties

Property code	Value	Unit	Source
gf	-174.74	kJ/mol	Joback Method
hf	-502.18	kJ/mol	Joback Method
hfus	41.65	kJ/mol	Joback Method
hvap	87.12	kJ/mol	Joback Method
log10ws	-6.22		Crippen Method
logp	4.825		Crippen Method
mcvol	258.170	ml/mol	McGowan Method
pc	1780.34	kPa	Joback Method
tb	892.43	K	Joback Method
tc	1122.94	K	Joback Method
tf	568.53	K	Joback Method
vc	0.981	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	744.88	J/molxK	892.43	Joback Method
cpg	757.38	J/molxK	930.85	Joback Method
cpg	768.61	J/molxK	969.27	Joback Method
cpg	778.59	J/molxK	1007.69	Joback Method
cpg	787.36	J/molxK	1046.11	Joback Method
cpg	794.94	J/molxK	1084.52	Joback Method
cpg	801.34	J/molxK	1122.94	Joback Method
dvisc	0.0003739	Paxs	568.53	Joback Method
dvisc	0.0002395	Paxs	622.51	Joback Method
dvisc	0.0001647	Paxs	676.50	Joback Method

dvisc	0.0001197	Paxs	730.48	Joback Method
dvisc	0.0000909	Paxs	784.46	Joback Method
dvisc	0.0000716	Paxs	838.45	Joback Method
dvisc	0.0000580	Paxs	892.43	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=U344591&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U344591&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>

## 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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