

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

<b>Inchi:</b>	InChI=1S/C18H17ClO4/c1-3-9-22-17(20)13-5-4-6-14(11-13)18(21)23-15-7-8-16(19)12(2)
<b>InchiKey:</b>	JZHAXCAOMKKXKC-UHFFFAOYSA-N
<b>Formula:</b>	C18H17ClO4
<b>SMILES:</b>	CCCOC(=O)c1cccc(C(=O)Oc2ccc(Cl)c(C)c2)c1
<b>Mol. weight [g/mol]:</b>	332.78

## Physical Properties

Property code	Value	Unit	Source
gf	-183.16	kJ/mol	Joback Method
hf	-481.54	kJ/mol	Joback Method
hfus	39.06	kJ/mol	Joback Method
hvap	84.90	kJ/mol	Joback Method
log10ws	-5.80		Crippen Method
logp	4.434		Crippen Method
mcvol	244.080	ml/mol	McGowan Method
pc	1933.83	kPa	Joback Method
tb	869.55	K	Joback Method
tc	1102.44	K	Joback Method
tf	557.26	K	Joback Method
vc	0.924	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	688.43	J/molxK	869.55	Joback Method
cpg	700.80	J/molxK	908.37	Joback Method
cpg	711.92	J/molxK	947.18	Joback Method
cpg	721.82	J/molxK	986.00	Joback Method
cpg	730.53	J/molxK	1024.81	Joback Method
cpg	738.05	J/molxK	1063.63	Joback Method
cpg	744.41	J/molxK	1102.44	Joback Method
dvisc	0.0004102	Paxs	557.26	Joback Method
dvisc	0.0002660	Paxs	609.31	Joback Method
dvisc	0.0001846	Paxs	661.36	Joback Method

dvisc	0.0001352	Paxs	713.40	Joback Method
dvisc	0.0001033	Paxs	765.45	Joback Method
dvisc	0.0000816	Paxs	817.50	Joback Method
dvisc	0.0000664	Paxs	869.55	Joback Method

## Sources

<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>
<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=U344589&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U344589&amp;Units=SI</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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