

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

Inchi:	InChI=1S/C17H15ClO4/c1-3-21-16(19)12-5-4-6-13(10-12)17(20)22-14-7-8-15(18)11(2)9-
InchiKey:	MSFVYZVUSJGPEG-UHFFFAOYSA-N
Formula:	C17H15ClO4
SMILES:	CCOC(=O)c1cccc(C(=O)Oc2ccc(Cl)c(C)c2)c1
Mol. weight [g/mol]:	318.75

## Physical Properties

Property code	Value	Unit	Source
gf	-191.58	kJ/mol	Joback Method
hf	-460.90	kJ/mol	Joback Method
hfus	36.47	kJ/mol	Joback Method
hvap	82.67	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	4.044		Crippen Method
mcvol	229.990	ml/mol	McGowan Method
pc	2108.07	kPa	Joback Method
rinpol	2574.00		NIST Webbook
rinpol	2574.00		NIST Webbook
tb	846.67	K	Joback Method
tc	1082.61	K	Joback Method
tf	545.99	K	Joback Method
vc	0.869	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	632.80	J/molxK	846.67	Joback Method
cpg	644.99	J/molxK	885.99	Joback Method
cpg	655.96	J/molxK	925.32	Joback Method
cpg	665.73	J/molxK	964.64	Joback Method
cpg	674.32	J/molxK	1003.97	Joback Method
cpg	681.75	J/molxK	1043.29	Joback Method
cpg	688.03	J/molxK	1082.61	Joback Method
dvisc	0.0004480	Paxs	545.99	Joback Method

dvisc	0.0002942	Paxs	596.10	Joback Method
dvisc	0.0002062	Paxs	646.22	Joback Method
dvisc	0.0001521	Paxs	696.33	Joback Method
dvisc	0.0001169	Paxs	746.44	Joback Method
dvisc	0.0000928	Paxs	796.56	Joback Method
dvisc	0.0000758	Paxs	846.67	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=U344588&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U344588&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>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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