

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

Inchi:	InChI=1S/C23H27ClO4/c1-3-4-5-6-7-8-14-27-22(25)18-10-9-11-19(16-18)23(26)28-20-12
InchiKey:	RJRQIYHAVUDKJY-UHFFFAOYSA-N
Formula:	C23H27ClO4
SMILES:	CCCCCCCCOC(=O)c1cccc(C(=O)Oc2ccc(Cl)c(C)c2)c1
Mol. weight [g/mol]:	402.91

## Physical Properties

Property code	Value	Unit	Source
gf	-141.06	kJ/mol	Joback Method
hf	-584.74	kJ/mol	Joback Method
hfus	52.01	kJ/mol	Joback Method
hvap	96.03	kJ/mol	Joback Method
log10ws	-7.89		Crippen Method
logp	6.385		Crippen Method
mcvol	314.530	ml/mol	McGowan Method
pc	1318.48	kPa	Joback Method
rinpol	3223.00		NIST Webbook
tb	983.95	K	Joback Method
tc	1212.54	K	Joback Method
tf	613.61	K	Joback Method
vc	1.204	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	977.51	J/molxK	983.95	Joback Method
cpg	1027.76	J/molxK	1174.44	Joback Method
cpg	1020.34	J/molxK	1136.34	Joback Method
cpg	1011.65	J/molxK	1098.25	Joback Method
cpg	1001.64	J/molxK	1060.15	Joback Method
cpg	990.27	J/molxK	1022.05	Joback Method
cpg	1033.93	J/molxK	1212.54	Joback Method
dvisc	0.0000329	Paxs	983.95	Joback Method
dvisc	0.0000411	Paxs	922.23	Joback Method

dvisc	0.0000531	Paxs	860.50	Joback Method
dvisc	0.0000714	Paxs	798.78	Joback Method
dvisc	0.0001009	Paxs	737.06	Joback Method
dvisc	0.0001519	Paxs	675.33	Joback Method
dvisc	0.0002483	Paxs	613.61	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=U344595&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U344595&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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