

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

<b>Inchi:</b>	InChI=1S/C24H29ClO4/c1-3-4-5-6-7-8-9-15-28-23(26)19-11-10-12-20(17-19)24(27)29-2
<b>InchiKey:</b>	UJNUHLUCULRGGG-UHFFFAOYSA-N
<b>Formula:</b>	C24H29ClO4
<b>SMILES:</b>	CCCCCCCCCOC(=O)c1cccc(C(=O)Oc2ccc(Cl)c(C)c2)c1
<b>Mol. weight [g/mol]:</b>	416.94

## Physical Properties

Property code	Value	Unit	Source
gf	-132.64	kJ/mol	Joback Method
hf	-605.38	kJ/mol	Joback Method
hfus	54.60	kJ/mol	Joback Method
hvap	98.25	kJ/mol	Joback Method
log10ws	-8.31		Crippen Method
logp	6.775		Crippen Method
mvol	328.620	ml/mol	McGowan Method
pc	1231.15	kPa	Joback Method
rinpol	3328.00		NIST Webbook
rinpol	3328.00		NIST Webbook
tb	1006.83	K	Joback Method
tc	1237.08	K	Joback Method
tf	624.88	K	Joback Method
vc	1.260	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1037.08	J/molxK	1006.83	Joback Method
cpg	1087.13	J/molxK	1198.70	Joback Method
cpg	1079.83	J/molxK	1160.33	Joback Method
cpg	1071.22	J/molxK	1121.95	Joback Method
cpg	1061.25	J/molxK	1083.58	Joback Method
cpg	1049.89	J/molxK	1045.20	Joback Method
cpg	1093.16	J/molxK	1237.08	Joback Method
dvisc	0.0000284	Paxs	1006.83	Joback Method

dvisc	0.0000356	Paxs	943.17	Joback Method
dvisc	0.0000462	Paxs	879.51	Joback Method
dvisc	0.0000624	Paxs	815.86	Joback Method
dvisc	0.0000887	Paxs	752.20	Joback Method
dvisc	0.0001345	Paxs	688.54	Joback Method
dvisc	0.0002222	Paxs	624.88	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=U344596&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U344596&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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