

# Isophthalic acid, 2,4-dichlorophenyl nonyl ester

Inchi:	InChI=1S/C23H26Cl2O4/c1-2-3-4-5-6-7-8-14-28-22(26)17-10-9-11-18(15-17)23(27)29-2
InchiKey:	CGRFUOSZZDPCMC-UHFFFAOYSA-N
Formula:	C23H26Cl2O4
SMILES:	CCCCCCCCCOC(=O)c1cccc(C(=O)Oc2ccc(Cl)cc2Cl)c1
Mol. weight [g/mol]:	437.36

## Physical Properties

Property code	Value	Unit	Source
gf	-152.99	kJ/mol	Joback Method
hf	-600.48	kJ/mol	Joback Method
hfus	56.21	kJ/mol	Joback Method
hvap	100.41	kJ/mol	Joback Method
log10ws	-8.52		Crippen Method
logp	7.120		Crippen Method
mvol	326.770	ml/mol	McGowan Method
pc	1283.75	kPa	Joback Method
rinpol	3344.00		NIST Webbook
rinpol	3344.00		NIST Webbook
tb	1021.38	K	Joback Method
tc	1255.57	K	Joback Method
tf	643.53	K	Joback Method
vc	1.254	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	998.18	J/molxK	1021.38	Joback Method
cpg	1009.59	J/molxK	1060.41	Joback Method
cpg	1019.59	J/molxK	1099.44	Joback Method
cpg	1028.24	J/molxK	1138.48	Joback Method
cpg	1035.58	J/molxK	1177.51	Joback Method
cpg	1041.66	J/molxK	1216.54	Joback Method
cpg	1046.53	J/molxK	1255.57	Joback Method
dvisc	0.0002042	Paxs	643.53	Joback Method

dvisc	0.0001263	Paxs	706.50	Joback Method
dvisc	0.0000845	Paxs	769.48	Joback Method
dvisc	0.0000601	Paxs	832.45	Joback Method
dvisc	0.0000448	Paxs	895.43	Joback Method
dvisc	0.0000348	Paxs	958.40	Joback Method
dvisc	0.0000278	Paxs	1021.38	Joback Method

## Sources

<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=U344413&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U344413&amp;Units=SI</a>
<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>

## Legend

<b>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</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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