

# Isophthalic acid, 3-methylpentyl nonyl ester

<b>Inchi:</b>	InChI=1S/C23H36O4/c1-4-6-7-8-9-10-11-16-26-22(24)20-13-12-14-21(18-20)23(25)27-1
<b>InchiKey:</b>	CXBPRRBQPSSFEC-UHFFFAOYSA-N
<b>Formula:</b>	C23H36O4
<b>SMILES:</b>	CCCCCCCCOC(=O)c1cccc(C(=O)OCCC(C)CC)c1
<b>Mol. weight [g/mol]:</b>	376.53

## Physical Properties

Property code	Value	Unit	Source
gf	-224.72	kJ/mol	Joback Method
hf	-787.87	kJ/mol	Joback Method
hfus	51.03	kJ/mol	Joback Method
hvap	87.65	kJ/mol	Joback Method
log10ws	-7.16		Crippen Method
logp	6.187		Crippen Method
mcvol	326.050	ml/mol	McGowan Method
pc	1103.74	kPa	Joback Method
rinpol	2735.00		NIST Webbook
tb	909.44	K	Joback Method
tc	1116.16	K	Joback Method
tf	517.23	K	Joback Method
vc	1.258	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1058.53	J/molxK	909.44	Joback Method
cpg	1075.35	J/molxK	943.89	Joback Method
cpg	1090.85	J/molxK	978.35	Joback Method
cpg	1105.07	J/molxK	1012.80	Joback Method
cpg	1118.04	J/molxK	1047.26	Joback Method
cpg	1129.80	J/molxK	1081.71	Joback Method
cpg	1140.38	J/molxK	1116.16	Joback Method
dvisc	0.0004827	Paxs	517.23	Joback Method
dvisc	0.0002394	Paxs	582.60	Joback Method

dvisc	0.0001368	Paxs	647.97	Joback Method
dvisc	0.0000866	Paxs	713.34	Joback Method
dvisc	0.0000592	Paxs	778.70	Joback Method
dvisc	0.0000429	Paxs	844.07	Joback Method
dvisc	0.0000326	Paxs	909.44	Joback Method

## Sources

<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=U356546&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356546&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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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