

# Isophthalic acid, 2-methylcyclohexyl nonyl ester

Inchi:	InChI=1S/C24H36O4/c1-3-4-5-6-7-8-11-17-27-23(25)20-14-12-15-21(18-20)24(26)28-22
InchiKey:	JBQVCXFMPBWSRL-UHFFFAOYSA-N
Formula:	C24H36O4
SMILES:	CCCCCCCCCOC(=O)c1cccc(C(=O)OC2CCCCC2C)c1
Mol. weight [g/mol]:	388.54

## Physical Properties

Property code	Value	Unit	Source
gf	-197.12	kJ/mol	Joback Method
hf	-769.25	kJ/mol	Joback Method
hfus	50.05	kJ/mol	Joback Method
hvap	90.39	kJ/mol	Joback Method
log10ws	-7.58		Crippen Method
logp	6.329		Crippen Method
mcvol	329.280	ml/mol	McGowan Method
pc	1155.35	kPa	Joback Method
rinpol	2982.00		NIST Webbook
rinpol	2982.00		NIST Webbook
tb	947.64	K	Joback Method
tc	1166.72	K	Joback Method
tf	546.64	K	Joback Method
vc	1.252	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1118.97	J/molxK	947.64	Joback Method
cpg	1135.90	J/molxK	984.15	Joback Method
cpg	1151.14	J/molxK	1020.67	Joback Method
cpg	1164.74	J/molxK	1057.18	Joback Method
cpg	1176.73	J/molxK	1093.70	Joback Method
cpg	1187.14	J/molxK	1130.21	Joback Method
cpg	1196.02	J/molxK	1166.72	Joback Method
dvisc	0.0004883	Paxs	546.64	Joback Method

dvisc	0.0002598	Paxs	613.47	Joback Method
dvisc	0.0001565	Paxs	680.31	Joback Method
dvisc	0.0001032	Paxs	747.14	Joback Method
dvisc	0.0000729	Paxs	813.97	Joback Method
dvisc	0.0000543	Paxs	880.81	Joback Method
dvisc	0.0000421	Paxs	947.64	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U345753&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U345753&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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