

# Phthalic acid, nonyl pent-4-enyl ester

<b>Inchi:</b>	InChI=1S/C22H32O4/c1-3-5-7-8-9-10-14-18-26-22(24)20-16-12-11-15-19(20)21(23)25-1
<b>InchiKey:</b>	KHIVFTSVFZEBQJ-UHFFFAOYSA-N
<b>Formula:</b>	C22H32O4
<b>SMILES:</b>	C=CCCCOC(=O)c1cccc1C(=O)OCCCCCCCC
<b>Mol. weight [g/mol]:</b>	360.49

## Physical Properties

Property code	Value	Unit	Source
gf	-142.86	kJ/mol	Joback Method
hf	-636.52	kJ/mol	Joback Method
hfus	50.68	kJ/mol	Joback Method
hvap	85.15	kJ/mol	Joback Method
log10ws	-6.83		Crippen Method
logp	5.717		Crippen Method
mvol	307.660	ml/mol	McGowan Method
pc	1205.63	kPa	Joback Method
rinpol	2550.00		NIST Webbook
tb	883.68	K	Joback Method
tc	1087.55	K	Joback Method
tf	519.20	K	Joback Method
vc	1.188	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	969.05	J/molxK	883.68	Joback Method
cpg	985.14	J/molxK	917.66	Joback Method
cpg	1000.05	J/molxK	951.64	Joback Method
cpg	1013.81	J/molxK	985.61	Joback Method
cpg	1026.45	J/molxK	1019.59	Joback Method
cpg	1038.00	J/molxK	1053.57	Joback Method
cpg	1048.51	J/molxK	1087.55	Joback Method
dvisc	0.0004940	Paxs	519.20	Joback Method
dvisc	0.0002678	Paxs	579.95	Joback Method

dvisc	0.0001630	Paxs	640.69	Joback Method
dvisc	0.0001082	Paxs	701.44	Joback Method
dvisc	0.0000766	Paxs	762.19	Joback Method
dvisc	0.0000571	Paxs	822.93	Joback Method
dvisc	0.0000443	Paxs	883.68	Joback Method

## Sources

<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=U360468&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U360468&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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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