

# Pimelic acid, 4-nitrophenyl nonyl ester

<b>Inchi:</b>	InChI=1S/C22H33NO6/c1-2-3-4-5-6-7-11-18-28-21(24)12-9-8-10-13-22(25)29-20-16-14-
<b>InchiKey:</b>	PXRZKYOBGSUPHA-UHFFFAOYSA-N
<b>Formula:</b>	C22H33NO6
<b>SMILES:</b>	CCCCCCCCCOC(=O)CCCCC(=O)Oc1ccc([N+](=O)[O-])cc1
<b>Mol. weight [g/mol]:</b>	407.50

## Physical Properties

Property code	Value	Unit	Source
gf	-195.15	kJ/mol	Joback Method
hf	-772.71	kJ/mol	Joback Method
hfus	63.32	kJ/mol	Joback Method
hvap	102.41	kJ/mol	Joback Method
log10ws	-7.16		Crippen Method
logp	5.744		Crippen Method
mvol	329.380	ml/mol	McGowan Method
pc	1180.90	kPa	Joback Method
rinpol	3198.00		NIST Webbook
rinpol	3198.00		NIST Webbook
tb	1038.84	K	Joback Method
tc	1271.93	K	Joback Method
tf	664.57	K	Joback Method
vc	1.290	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1108.40	J/mol×K	1038.84	Joback Method
cpg	1121.22	J/mol×K	1077.69	Joback Method
cpg	1132.57	J/mol×K	1116.54	Joback Method
cpg	1142.47	J/mol×K	1155.39	Joback Method
cpg	1150.99	J/mol×K	1194.23	Joback Method
cpg	1158.17	J/mol×K	1233.08	Joback Method
cpg	1164.06	J/mol×K	1271.93	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=U416623&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U416623&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<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>hvp:</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>rinp:</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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