

# Sebacic acid, 4-nitrophenyl nonyl ester

<b>Inchi:</b>	InChI=1S/C25H39NO6/c1-2-3-4-5-8-11-14-21-31-24(27)15-12-9-6-7-10-13-16-25(28)32-
<b>InchiKey:</b>	RIDNIQINGBXNAQ-UHFFFAOYSA-N
<b>Formula:</b>	C25H39NO6
<b>SMILES:</b>	CCCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1ccc([N+](=O)[O-])cc1
<b>Mol. weight [g/mol]:</b>	449.58

## Physical Properties

Property code	Value	Unit	Source
gf	-169.89	kJ/mol	Joback Method
hf	-834.63	kJ/mol	Joback Method
hfus	71.09	kJ/mol	Joback Method
hvap	109.08	kJ/mol	Joback Method
log10ws	-8.41		Crippen Method
logp	6.915		Crippen Method
mcvol	371.650	ml/mol	McGowan Method
pc	977.78	kPa	Joback Method
rinpol	3574.00		NIST Webbook
tb	1107.48	K	Joback Method
tc	1359.81	K	Joback Method
tf	698.38	K	Joback Method
vc	1.458	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1291.28	J/mol×K	1107.48	Joback Method
cpg	1304.53	J/mol×K	1149.54	Joback Method
cpg	1316.00	J/mol×K	1191.59	Joback Method
cpg	1325.78	J/mol×K	1233.65	Joback Method
cpg	1333.94	J/mol×K	1275.70	Joback Method
cpg	1340.56	J/mol×K	1317.76	Joback Method
cpg	1345.73	J/mol×K	1359.81	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=U354792&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354792&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>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>mccvol:</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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