

# Sebacic acid, nonyl pent-4-enyl ester

<b>Inchi:</b>	InChI=1S/C24H44O4/c1-3-5-7-8-11-14-18-22-28-24(26)20-16-13-10-9-12-15-19-23(25)2
<b>InchiKey:</b>	QDSSEGXRKGHUMA-UHFFFAOYSA-N
<b>Formula:</b>	C24H44O4
<b>SMILES:</b>	C=CCCCOC(=O)CCCCCCCCC(=O)OCCCCCCCCC
<b>Mol. weight [g/mol]:</b>	396.60

## Physical Properties

Property code	Value	Unit	Source
gf	-228.80	kJ/mol	Joback Method
hf	-902.86	kJ/mol	Joback Method
hfus	62.21	kJ/mol	Joback Method
hvap	86.66	kJ/mol	Joback Method
log10ws	-7.45		Crippen Method
logp	6.910		Crippen Method
mcvol	359.600	ml/mol	McGowan Method
pc	871.19	kPa	Joback Method
rinsol	2779.00		NIST Webbook
tb	897.78	K	Joback Method
tc	1099.94	K	Joback Method
tf	502.80	K	Joback Method
vc	1.409	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1188.70	J/molxK	897.78	Joback Method
cpg	1208.28	J/molxK	931.47	Joback Method
cpg	1226.53	J/molxK	965.17	Joback Method
cpg	1243.49	J/molxK	998.86	Joback Method
cpg	1259.19	J/molxK	1032.56	Joback Method
cpg	1273.67	J/molxK	1066.25	Joback Method
cpg	1286.97	J/molxK	1099.94	Joback Method
dvisc	0.0005395	Paxs	502.80	Joback Method
dvisc	0.0002558	Paxs	568.63	Joback Method

dvisc	0.0001416	Paxs	634.46	Joback Method
dvisc	0.0000876	Paxs	700.29	Joback Method
dvisc	0.0000588	Paxs	766.12	Joback Method
dvisc	0.0000421	Paxs	831.95	Joback Method
dvisc	0.0000316	Paxs	897.78	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=U355415&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355415&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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