

# Sebacic acid, 2,4-dimethylpent-3-yl nonyl ester

<b>Inchi:</b>	InChI=1S/C26H50O4/c1-6-7-8-9-12-15-18-21-29-24(27)19-16-13-10-11-14-17-20-25(28)
<b>InchiKey:</b>	FLAQPHIVZAXYSK-UHFFFAOYSA-N
<b>Formula:</b>	C26H50O4
<b>SMILES:</b>	CCCCCCCCCOC(=O)CCCCCCCCC(=O)OC(C(C)C)C(C)C
<b>Mol. weight [g/mol]:</b>	426.67

## Physical Properties

Property code	Value	Unit	Source
gf	-307.12	kJ/mol	Joback Method
hf	-1085.41	kJ/mol	Joback Method
hfus	58.10	kJ/mol	Joback Method
hvap	90.62	kJ/mol	Joback Method
log10ws	-8.06		Crippen Method
logp	7.625		Crippen Method
mvol	392.080	ml/mol	McGowan Method
pc	772.46	kPa	Joback Method
rinpol	2824.00		NIST Webbook
rinpol	2824.00		NIST Webbook
tb	945.54	K	Joback Method
tc	1161.05	K	Joback Method
tf	482.10	K	Joback Method
vc	1.522	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1346.32	J/molxK	945.54	Joback Method
cpg	1434.66	J/molxK	1125.13	Joback Method
cpg	1420.12	J/molxK	1089.21	Joback Method
cpg	1404.07	J/molxK	1053.29	Joback Method
cpg	1386.45	J/molxK	1017.38	Joback Method
cpg	1367.21	J/molxK	981.46	Joback Method
cpg	1447.72	J/molxK	1161.05	Joback Method
dvisc	0.0000164	Paxs	945.54	Joback Method

dvisc	0.0000230	Paxs	868.30	Joback Method
dvisc	0.0000345	Paxs	791.06	Joback Method
dvisc	0.0000565	Paxs	713.82	Joback Method
dvisc	0.0001044	Paxs	636.58	Joback Method
dvisc	0.0002284	Paxs	559.34	Joback Method
dvisc	0.0006421	Paxs	482.10	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=U355432&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355432&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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