

# Sebacic acid, 3-methylbut-2-yl nonyl ester

<b>Inchi:</b>	InChI=1S/C24H46O4/c1-5-6-7-8-11-14-17-20-27-23(25)18-15-12-9-10-13-16-19-24(26)2
<b>InchiKey:</b>	SHLOXMWTXMWLOF-UHFFFAOYSA-N
<b>Formula:</b>	C24H46O4
<b>SMILES:</b>	CCCCCCCCCOC(=O)CCCCCCCCC(=O)OC(C)C(C)C
<b>Mol. weight [g/mol]:</b>	398.62

## Physical Properties

Property code	Value	Unit	Source
gf	-321.52	kJ/mol	Joback Method
hf	-1038.85	kJ/mol	Joback Method
hfus	56.44	kJ/mol	Joback Method
hvap	86.55	kJ/mol	Joback Method
log10ws	-7.46		Crippen Method
logp	6.989		Crippen Method
mvol	363.900	ml/mol	McGowan Method
pc	857.97	kPa	Joback Method
rinpol	2688.00		NIST Webbook
tb	900.22	K	Joback Method
tc	1102.59	K	Joback Method
tf	474.56	K	Joback Method
vc	1.415	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1218.42	J/molxK	900.22	Joback Method
cpg	1238.45	J/molxK	933.95	Joback Method
cpg	1257.07	J/molxK	967.68	Joback Method
cpg	1274.32	J/molxK	1001.41	Joback Method
cpg	1290.22	J/molxK	1035.14	Joback Method
cpg	1304.81	J/molxK	1068.86	Joback Method
cpg	1318.12	J/molxK	1102.59	Joback Method
dvisc	0.0007142	Paxs	474.56	Joback Method
dvisc	0.0002826	Paxs	545.50	Joback Method

dvisc	0.0001385	Paxs	616.45	Joback Method
dvisc	0.0000786	Paxs	687.39	Joback Method
dvisc	0.0000496	Paxs	758.33	Joback Method
dvisc	0.0000339	Paxs	829.28	Joback Method
dvisc	0.0000246	Paxs	900.22	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=U355565&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355565&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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