

# Sebacic acid, 4-methoxybenzyl nonyl ester

<b>Inchi:</b>	InChI=1S/C27H44O5/c1-3-4-5-6-9-12-15-22-31-26(28)16-13-10-7-8-11-14-17-27(29)32-2
<b>InchiKey:</b>	DZASNAJABIKVRV-UHFFFAOYSA-N
<b>Formula:</b>	C27H44O5
<b>SMILES:</b>	CCCCCCCCCOC(=O)CCCCCCCCC(=O)OCc1ccc(OC)cc1
<b>Mol. weight [g/mol]:</b>	448.64

## Physical Properties

Property code	Value	Unit	Source
gf	-293.60	kJ/mol	Joback Method
hf	-997.37	kJ/mol	Joback Method
hfus	66.10	kJ/mol	Joback Method
hvap	99.36	kJ/mol	Joback Method
log10ws	-8.15		Crippen Method
logp	7.153		Crippen Method
mcvol	388.280	ml/mol	McGowan Method
pc	855.46	kPa	Joback Method
rinpola	3421.00		NIST Webbook
tb	1023.82	K	Joback Method
tc	1258.07	K	Joback Method
tf	599.54	K	Joback Method
vc	1.506	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1335.61	J/molxK	1023.82	Joback Method
cpg	1401.98	J/molxK	1219.03	Joback Method
cpg	1392.36	J/molxK	1179.99	Joback Method
cpg	1380.96	J/molxK	1140.94	Joback Method
cpg	1367.73	J/molxK	1101.90	Joback Method
cpg	1352.63	J/molxK	1062.86	Joback Method
cpg	1409.86	J/molxK	1258.07	Joback Method
dvisc	0.0000144	Paxs	1023.82	Joback Method
dvisc	0.0000188	Paxs	953.11	Joback Method

dvisc	0.0000256	Paxs	882.39	Joback Method
dvisc	0.0000369	Paxs	811.68	Joback Method
dvisc	0.0000569	Paxs	740.97	Joback Method
dvisc	0.0000963	Paxs	670.25	Joback Method
dvisc	0.0001845	Paxs	599.54	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<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=U354368&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354368&amp;Units=SI</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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