

# Sebacic acid, nonyl 3-phenylallyl ester

<b>Inchi:</b>	InChI=1S/C28H44O4/c1-2-3-4-5-8-11-17-24-31-27(29)22-15-9-6-7-10-16-23-28(30)32-25
<b>InchiKey:</b>	HVYBMHPGNHEPFL-DYTRJAOYSA-N
<b>Formula:</b>	C28H44O4
<b>SMILES:</b>	CCCCCCCCCOC(=O)CCCCCCCCC(=O)OCC=Cc1ccccc1
<b>Mol. weight [g/mol]:</b>	444.65

## Physical Properties

Property code	Value	Unit	Source
gf	-90.33	kJ/mol	Joback Method
hf	-757.10	kJ/mol	Joback Method
hfus	68.09	kJ/mol	Joback Method
hvap	98.47	kJ/mol	Joback Method
log10ws	-8.39		Crippen Method
logp	7.658		Crippen Method
mvol	392.200	ml/mol	McGowan Method
pc	849.49	kPa	Joback Method
rinpol	3412.00		NIST Webbook
rinpol	3412.00		NIST Webbook
tb	1023.46	K	Joback Method
tc	1255.93	K	Joback Method
tf	570.98	K	Joback Method
vc	1.524	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1341.57	J/molxK	1023.46	Joback Method
cpg	1359.71	J/molxK	1062.20	Joback Method
cpg	1376.35	J/molxK	1100.95	Joback Method
cpg	1391.56	J/molxK	1139.69	Joback Method
cpg	1405.46	J/molxK	1178.44	Joback Method
cpg	1418.11	J/molxK	1217.18	Joback Method
cpg	1429.64	J/molxK	1255.93	Joback Method
dvisc	0.0002504	Paxs	570.98	Joback Method

dvisc	0.0001177	Paxs	646.39	Joback Method
dvisc	0.0000648	Paxs	721.81	Joback Method
dvisc	0.0000399	Paxs	797.22	Joback Method
dvisc	0.0000268	Paxs	872.63	Joback Method
dvisc	0.0000191	Paxs	948.05	Joback Method
dvisc	0.0000143	Paxs	1023.46	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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=U355895&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355895&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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