

# Sebacic acid, octyl 3-phenylpropyl ester

**Inchi:** InChI=1S/C27H44O4/c1-2-3-4-5-10-16-23-30-26(28)21-14-8-6-7-9-15-22-27(29)31-24-17  
**InchiKey:** AALHMANQUJIXOP-UHFFFAOYSA-N  
**Formula:** C27H44O4  
**SMILES:** CCCCCCOC(=O)CCCCCCCC(=O)OCCc1ccccc1  
**Mol. weight [g/mol]:** 432.64

## Physical Properties

Property code	Value	Unit	Source
gf	-178.97	kJ/mol	Joback Method
hf	-853.68	kJ/mol	Joback Method
hfus	65.30	kJ/mol	Joback Method
hvap	96.28	kJ/mol	Joback Method
log10ws	-7.95		Crippen Method
logp	7.187		Crippen Method
mvol	382.410	ml/mol	McGowan Method
pc	871.71	kPa	Joback Method
rinpol	3298.00		NIST Webbook
tb	996.42	K	Joback Method
tc	1221.91	K	Joback Method
tf	564.79	K	Joback Method
vc	1.488	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1307.01	J/molxK	996.42	Joback Method
cpg	1325.04	J/molxK	1034.00	Joback Method
cpg	1341.46	J/molxK	1071.58	Joback Method
cpg	1356.33	J/molxK	1109.17	Joback Method
cpg	1369.72	J/molxK	1146.75	Joback Method
cpg	1381.69	J/molxK	1184.33	Joback Method
cpg	1392.31	J/molxK	1221.91	Joback Method
dvisc	0.0003070	Paxs	564.79	Joback Method
dvisc	0.0001487	Paxs	636.73	Joback Method

dvisc	0.0000835	Paxs	708.67	Joback Method
dvisc	0.0000521	Paxs	780.61	Joback Method
dvisc	0.0000352	Paxs	852.54	Joback Method
dvisc	0.0000253	Paxs	924.48	Joback Method
dvisc	0.0000191	Paxs	996.42	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=U354392&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354392&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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