

# Sebacic acid, octyl 3-propylphenyl ester

**Inchi:** InChI=1S/C27H44O4/c1-3-5-6-7-12-17-23-30-26(28)21-13-10-8-9-11-14-22-27(29)31-25  
**InchiKey:** KBZSARWIIWXJIU-UHFFFAOYSA-N  
**Formula:** C27H44O4  
**SMILES:** CCCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1ccccc1CCC  
**Mol. weight [g/mol]:** 432.64

## Physical Properties

Property code	Value	Unit	Source
gf	-188.60	kJ/mol	Joback Method
hf	-865.15	kJ/mol	Joback Method
hfus	64.91	kJ/mol	Joback Method
hvap	96.95	kJ/mol	Joback Method
log10ws	-8.57		Crippen Method
logp	7.569		Crippen Method
mcvol	382.410	ml/mol	McGowan Method
pc	864.04	kPa	Joback Method
rinpol	3133.00		NIST Webbook
tb	1001.40	K	Joback Method
tc	1228.17	K	Joback Method
tf	577.31	K	Joback Method
vc	1.488	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1306.45	J/molxK	1001.40	Joback Method
cpg	1379.97	J/molxK	1190.37	Joback Method
cpg	1368.34	J/molxK	1152.58	Joback Method
cpg	1355.23	J/molxK	1114.78	Joback Method
cpg	1340.59	J/molxK	1076.99	Joback Method
cpg	1324.35	J/molxK	1039.19	Joback Method
cpg	1390.19	J/molxK	1228.17	Joback Method
dvisc	0.0000195	Paxs	1001.40	Joback Method
dvisc	0.0000256	Paxs	930.72	Joback Method

dvisc	0.0000351	Paxs	860.04	Joback Method
dvisc	0.0000510	Paxs	789.36	Joback Method
dvisc	0.0000795	Paxs	718.67	Joback Method
dvisc	0.0001367	Paxs	647.99	Joback Method
dvisc	0.0002685	Paxs	577.31	Joback Method

## Sources

<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=U355056&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355056&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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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