

# Sebacic acid, hex-4-yn-3-yl undecyl ester

**Inchi:** InChI=1S/C27H48O4/c1-4-7-8-9-10-11-14-17-20-24-30-26(28)22-18-15-12-13-16-19-23-  
**InchiKey:** KLOVZEVLUNZWPN-UHFFFAOYSA-N  
**Formula:** C27H48O4  
**SMILES:** CC#CC(CC)OC(=O)CCCCCCCCC(=O)OCCCCCCCCCCC  
**Mol. weight [g/mol]:** 436.67

## Physical Properties

Property code	Value	Unit	Source
gf	-91.02	kJ/mol	Joback Method
hf	-823.19	kJ/mol	Joback Method
hfus	70.86	kJ/mol	Joback Method
hvap	95.77	kJ/mol	Joback Method
log10ws	-8.76		Crippen Method
logp	7.526		Crippen Method
mcvol	397.570	ml/mol	McGowan Method
pc	793.49	kPa	Joback Method
rinqol	3023.00		NIST Webbook
tb	978.30	K	Joback Method
tc	1201.23	K	Joback Method
tf	629.47	K	Joback Method
vc	1.552	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1354.91	J/molxK	978.30	Joback Method
cpg	1374.81	J/molxK	1015.46	Joback Method
cpg	1393.05	J/molxK	1052.61	Joback Method
cpg	1409.66	J/molxK	1089.77	Joback Method
cpg	1424.69	J/molxK	1126.92	Joback Method
cpg	1438.20	J/molxK	1164.08	Joback Method
cpg	1450.23	J/molxK	1201.23	Joback Method

# Sources

<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=U355828&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355828&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<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>rinpola:</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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