

# Sebacic acid, 2,7-dimethylocta-7-en-5-yn-4-yl hexyl ester

<b>Inchi:</b>	InChI=1S/C26H44O4/c1-6-7-8-15-20-29-25(27)16-13-11-9-10-12-14-17-26(28)30-24(21-
<b>InchiKey:</b>	QENMDAFWCNSMBD-UHFFFAOYSA-N
<b>Formula:</b>	C26H44O4
<b>SMILES:</b>	C=C(C)C#CC(CC(C)C)OC(=O)CCCCCCCC(=O)OCCCCC
<b>Mol. weight [g/mol]:</b>	420.63

## Physical Properties

Property code	Value	Unit	Source
gf	-22.59	kJ/mol	Joback Method
hf	-692.19	kJ/mol	Joback Method
hfus	62.16	kJ/mol	Joback Method
hvap	92.57	kJ/mol	Joback Method
log10ws	-7.95		Crippen Method
logp	6.768		Crippen Method
mvol	379.180	ml/mol	McGowan Method
pc	865.56	kPa	Joback Method
rinpol	2728.00		NIST Webbook
rinpol	2728.00		NIST Webbook
tb	951.54	K	Joback Method
tc	1165.04	K	Joback Method
tf	587.48	K	Joback Method
vc	1.472	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1261.56	J/mol×K	951.54	Joback Method
cpg	1280.43	J/mol×K	987.12	Joback Method
cpg	1297.86	J/mol×K	1022.71	Joback Method
cpg	1313.87	J/mol×K	1058.29	Joback Method
cpg	1328.52	J/mol×K	1093.87	Joback Method
cpg	1341.86	J/mol×K	1129.46	Joback Method
cpg	1353.92	J/mol×K	1165.04	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=U355817&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355817&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.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>

# 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>h vap:</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>r in pol:</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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