

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

**Inchi:** InChI=1S/C24H40O4/c1-6-7-18-27-23(25)14-12-10-8-9-11-13-15-24(26)28-22(19-21(4)5)  
**InchiKey:** LGOIFMFYBFANRW-UHFFFAOYSA-N  
**Formula:** C24H40O4  
**SMILES:** C=C(C)C#CC(CC(C)C)OC(=O)CCCCCCCC(=O)OCCCC  
**Mol. weight [g/mol]:** 392.57

## Physical Properties

Property code	Value	Unit	Source
gf	-39.43	kJ/mol	Joback Method
hf	-650.91	kJ/mol	Joback Method
hfus	56.98	kJ/mol	Joback Method
hvap	88.12	kJ/mol	Joback Method
log10ws	-7.11		Crippen Method
logp	5.988		Crippen Method
mvol	351.000	ml/mol	McGowan Method
pc	972.30	kPa	Joback Method
rinpol	2549.00		NIST Webbook
rinpol	2549.00		NIST Webbook
tb	905.78	K	Joback Method
tc	1110.14	K	Joback Method
tf	564.94	K	Joback Method
vc	1.359	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1136.37	J/mol×K	905.78	Joback Method
cpg	1154.62	J/mol×K	939.84	Joback Method
cpg	1171.58	J/mol×K	973.90	Joback Method
cpg	1187.28	J/mol×K	1007.96	Joback Method
cpg	1201.76	J/mol×K	1042.02	Joback Method
cpg	1215.06	J/mol×K	1076.08	Joback Method
cpg	1227.20	J/mol×K	1110.14	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.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=U355815&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355815&amp;Units=SI</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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