

# Sebacic acid, heptyl 2-methyloct-5-yn-4-yl ester

Inchi:	InChI=1S/C26H46O4/c1-5-7-9-14-17-21-29-25(27)19-15-12-10-11-13-16-20-26(28)30-24
InchiKey:	GLVPXUHDTOKNHL-UHFFFAOYSA-N
Formula:	C26H46O4
SMILES:	CCC#CC(CC(C)C)OC(=O)CCCCCCCCC(=O)OCCCCCCC
Mol. weight [g/mol]:	422.64

## Physical Properties

Property code	Value	Unit	Source
gf	-101.88	kJ/mol	Joback Method
hf	-807.83	kJ/mol	Joback Method
hfus	64.75	kJ/mol	Joback Method
hvap	93.16	kJ/mol	Joback Method
log10ws	-8.10		Crippen Method
logp	6.992		Crippen Method
mcvol	383.480	ml/mol	McGowan Method
pc	842.11	kPa	Joback Method
rinqol	2799.00		NIST Webbook
tb	954.98	K	Joback Method
tc	1169.90	K	Joback Method
tf	603.20	K	Joback Method
vc	1.490	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1291.58	J/molxK	954.98	Joback Method
cpg	1310.96	J/molxK	990.80	Joback Method
cpg	1328.79	J/molxK	1026.62	Joback Method
cpg	1345.11	J/molxK	1062.44	Joback Method
cpg	1359.96	J/molxK	1098.26	Joback Method
cpg	1373.38	J/molxK	1134.08	Joback Method
cpg	1385.42	J/molxK	1169.90	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=U355871&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355871&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>

# 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>hvac:</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>mccol:</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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