

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

<b>Inchi:</b>	InChI=1S/C24H42O4/c1-5-7-15-19-27-23(25)17-13-11-9-10-12-14-18-24(26)28-22(16-8-
<b>InchiKey:</b>	MVZSWVXKWIIMOW-UHFFFAOYSA-N
<b>Formula:</b>	C24H42O4
<b>SMILES:</b>	CCC#CC(CC(C)C)OC(=O)CCCCCCCCC(=O)OCCCCC
<b>Mol. weight [g/mol]:</b>	394.59

## Physical Properties

Property code	Value	Unit	Source
gf	-118.72	kJ/mol	Joback Method
hf	-766.55	kJ/mol	Joback Method
hfus	59.57	kJ/mol	Joback Method
hvap	88.71	kJ/mol	Joback Method
log10ws	-7.26		Crippen Method
logp	6.212		Crippen Method
mvol	355.300	ml/mol	McGowan Method
pc	944.42	kPa	Joback Method
rinpol	2605.00		NIST Webbook
rinpol	2605.00		NIST Webbook
tb	909.22	K	Joback Method
tc	1113.45	K	Joback Method
tf	580.66	K	Joback Method
vc	1.377	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1165.63	J/molxK	909.22	Joback Method
cpg	1184.33	J/molxK	943.26	Joback Method
cpg	1201.67	J/molxK	977.30	Joback Method
cpg	1217.69	J/molxK	1011.34	Joback Method
cpg	1232.42	J/molxK	1045.37	Joback Method
cpg	1245.89	J/molxK	1079.41	Joback Method
cpg	1258.12	J/molxK	1113.45	Joback Method

# Sources

<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=U355870&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355870&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>

# 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>hvp:</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>rinp:</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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