

# Sebacic acid, but-3-yn-2-yl decyl ester

<b>Inchi:</b>	InChI=1S/C24H42O4/c1-4-6-7-8-9-12-15-18-21-27-23(25)19-16-13-10-11-14-17-20-24(2
<b>InchiKey:</b>	GPFHGULGBDHUFM-UHFFFAOYSA-N
<b>Formula:</b>	C24H42O4
<b>SMILES:</b>	C#CC(C)OC(=O)CCCCCCCCC(=O)OCCCCCCCCC
<b>Mol. weight [g/mol]:</b>	394.59

## Physical Properties

Property code	Value	Unit	Source
gf	-96.01	kJ/mol	Joback Method
hf	-741.67	kJ/mol	Joback Method
hfus	62.94	kJ/mol	Joback Method
hvap	86.80	kJ/mol	Joback Method
log10ws	-7.50		Crippen Method
logp	6.356		Crippen Method
mvol	355.300	ml/mol	McGowan Method
pc	932.92	kPa	Joback Method
rmpol	2678.00		NIST Webbook
tb	890.78	K	Joback Method
tc	1090.57	K	Joback Method
tf	536.53	K	Joback Method
vc	1.383	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1158.20	J/mol×K	890.78	Joback Method
cpg	1177.05	J/mol×K	924.08	Joback Method
cpg	1194.65	J/mol×K	957.38	Joback Method
cpg	1211.03	J/mol×K	990.68	Joback Method
cpg	1226.24	J/mol×K	1023.97	Joback Method
cpg	1240.29	J/mol×K	1057.27	Joback Method
cpg	1253.24	J/mol×K	1090.57	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=U355852&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355852&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>

# 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>hvpap:</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>mccvol:</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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