

# Sebacic acid, but-3-enyl dodecyl ester

**Inchi:** InChI=1S/C26H48O4/c1-3-5-7-8-9-10-11-14-17-20-24-30-26(28)22-19-16-13-12-15-18-2  
**InchiKey:** TWAMPNVGXDKUBN-UHFFFAOYSA-N  
**Formula:** C26H48O4  
**SMILES:** C=CCCOC(=O)CCCCCCCCC(=O)OCCCCCCCCCCCCC  
**Mol. weight [g/mol]:** 424.66

## Physical Properties

Property code	Value	Unit	Source
gf	-211.96	kJ/mol	Joback Method
hf	-944.14	kJ/mol	Joback Method
hfus	67.39	kJ/mol	Joback Method
hvap	91.11	kJ/mol	Joback Method
log10ws	-8.28		Crippen Method
logp	7.691		Crippen Method
mvol	387.780	ml/mol	McGowan Method
pc	780.25	kPa	Joback Method
rinpol	2969.00		NIST Webbook
rinpol	2969.00		NIST Webbook
tb	943.54	K	Joback Method
tc	1160.67	K	Joback Method
tf	525.34	K	Joback Method
vc	1.520	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1315.55	J/molxK	943.54	Joback Method
cpg	1404.04	J/molxK	1124.48	Joback Method
cpg	1389.28	J/molxK	1088.30	Joback Method
cpg	1373.10	J/molxK	1052.11	Joback Method
cpg	1355.46	J/molxK	1015.92	Joback Method
cpg	1336.29	J/molxK	979.73	Joback Method
cpg	1417.43	J/molxK	1160.67	Joback Method
dvisc	0.0000233	Paxs	943.54	Joback Method

dvisc	0.0000312	Paxs	873.84	Joback Method
dvisc	0.0000438	Paxs	804.14	Joback Method
dvisc	0.0000656	Paxs	734.44	Joback Method
dvisc	0.0001071	Paxs	664.74	Joback Method
dvisc	0.0001960	Paxs	595.04	Joback Method
dvisc	0.0004211	Paxs	525.34	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=U356092&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356092&amp;Units=SI</a>
<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.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>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mcvol:</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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