

# Sebacic acid, but-3-enyl tridecyl ester

**Inchi:** InChI=1S/C27H50O4/c1-3-5-7-8-9-10-11-12-15-18-21-25-31-27(29)23-20-17-14-13-16-1  
**InchiKey:** KRCBCIOPPZVENH-UHFFFAOYSA-N  
**Formula:** C27H50O4  
**SMILES:** C=CCCOC(=O)CCCCCCCCC(=O)OCCCCCCCCCCCCC  
**Mol. weight [g/mol]:** 438.68

## Physical Properties

Property code	Value	Unit	Source
gf	-203.54	kJ/mol	Joback Method
hf	-964.78	kJ/mol	Joback Method
hfus	69.98	kJ/mol	Joback Method
hvap	93.34	kJ/mol	Joback Method
log10ws	-8.70		Crippen Method
logp	8.081		Crippen Method
mvol	401.870	ml/mol	McGowan Method
pc	740.03	kPa	Joback Method
rinpol	3069.00		NIST Webbook
rinpol	3069.00		NIST Webbook
tb	966.42	K	Joback Method
tc	1192.80	K	Joback Method
tf	536.61	K	Joback Method
vc	1.577	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1379.69	J/molxK	966.42	Joback Method
cpg	1470.03	J/molxK	1155.07	Joback Method
cpg	1455.15	J/molxK	1117.34	Joback Method
cpg	1438.75	J/molxK	1079.61	Joback Method
cpg	1420.75	J/molxK	1041.88	Joback Method
cpg	1401.08	J/molxK	1004.15	Joback Method
cpg	1483.43	J/molxK	1192.80	Joback Method
dvisc	0.0000200	Paxs	966.42	Joback Method

dvisc	0.0000267	Paxs	894.79	Joback Method
dvisc	0.0000377	Paxs	823.15	Joback Method
dvisc	0.0000566	Paxs	751.52	Joback Method
dvisc	0.0000928	Paxs	679.88	Joback Method
dvisc	0.0001709	Paxs	608.25	Joback Method
dvisc	0.0003705	Paxs	536.61	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=U356093&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356093&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>dvisc:</b>	Dynamic viscosity
<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>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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