

# Sebacic acid, but-2-enyl nonyl ester

<b>Inchi:</b>	InChI=1S/C23H42O4/c1-3-5-7-8-11-14-17-21-27-23(25)19-16-13-10-9-12-15-18-22(24)2
<b>InchiKey:</b>	PMPFWULFWQBPFJ-GQCTYLIASA-N
<b>Formula:</b>	C23H42O4
<b>SMILES:</b>	CC=CCOC(=O)CCCCCCCCC(=O)OCCCCCCCCC
<b>Mol. weight [g/mol]:</b>	382.58

## Physical Properties

Property code	Value	Unit	Source
gf	-244.84	kJ/mol	Joback Method
hf	-890.43	kJ/mol	Joback Method
hfus	61.10	kJ/mol	Joback Method
hvap	85.06	kJ/mol	Joback Method
log10ws	-7.03		Crippen Method
logp	6.520		Crippen Method
mcvol	345.510	ml/mol	McGowan Method
pc	928.37	kPa	Joback Method
rinpol	2681.00		NIST Webbook
rinpol	2681.00		NIST Webbook
tb	882.38	K	Joback Method
tc	1080.29	K	Joback Method
tf	488.21	K	Joback Method
vc	1.351	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1127.87	J/molxK	882.38	Joback Method
cpg	1211.47	J/molxK	1047.30	Joback Method
cpg	1197.00	J/molxK	1014.32	Joback Method
cpg	1181.44	J/molxK	981.33	Joback Method
cpg	1164.75	J/molxK	948.35	Joback Method
cpg	1146.91	J/molxK	915.36	Joback Method
cpg	1224.91	J/molxK	1080.29	Joback Method
dvisc	0.0000299	Paxs	882.38	Joback Method

dvisc	0.0000400	Paxs	816.68	Joback Method
dvisc	0.0000562	Paxs	750.99	Joback Method
dvisc	0.0000845	Paxs	685.30	Joback Method
dvisc	0.0001384	Paxs	619.60	Joback Method
dvisc	0.0002548	Paxs	553.90	Joback Method
dvisc	0.0005530	Paxs	488.21	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=U354310&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354310&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>rlnpol:</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

Latest version available from:

<https://www.chemeo.com/cid/57-543-6/Sebacic-acid-but-2-enyl-nonyl-ester.pdf>

Generated by Cheméo on 2024-04-30 04:55:41.244854801 +0000 UTC m=+16742190.165432137.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.