

# Sebacic acid, hexyl oct-3-en-2-yl ester

<b>Inchi:</b>	InChI=1S/C24H44O4/c1-4-6-8-14-18-22(3)28-24(26)20-16-13-11-10-12-15-19-23(25)27-
<b>InchiKey:</b>	KTIGMJSPCKGHGB-NBVRZTHBSA-N
<b>Formula:</b>	C24H44O4
<b>SMILES:</b>	CCCCC=CC(C)OC(=O)CCCCCCCC(=O)OCCCCC
<b>Mol. weight [g/mol]:</b>	396.60

## Physical Properties

Property code	Value	Unit	Source
gf	-238.86	kJ/mol	Joback Method
hf	-916.35	kJ/mol	Joback Method
hfus	60.17	kJ/mol	Joback Method
hvap	86.90	kJ/mol	Joback Method
log10ws	-7.56		Crippen Method
logp	6.909		Crippen Method
mcvol	359.600	ml/mol	McGowan Method
pc	880.52	kPa	Joback Method
rinqol	2662.00		NIST Webbook
tb	904.82	K	Joback Method
tc	1108.02	K	Joback Method
tf	484.48	K	Joback Method
vc	1.401	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1190.97	J/molxK	904.82	Joback Method
cpg	1210.47	J/molxK	938.69	Joback Method
cpg	1228.67	J/molxK	972.55	Joback Method
cpg	1245.63	J/molxK	1006.42	Joback Method
cpg	1261.38	J/molxK	1040.29	Joback Method
cpg	1275.97	J/molxK	1074.15	Joback Method
cpg	1289.45	J/molxK	1108.02	Joback Method
dvisc	0.0005674	Paxs	484.48	Joback Method
dvisc	0.0002387	Paxs	554.54	Joback Method

dvisc	0.0001219	Paxs	624.59	Joback Method
dvisc	0.0000713	Paxs	694.65	Joback Method
dvisc	0.0000460	Paxs	764.71	Joback Method
dvisc	0.0000320	Paxs	834.76	Joback Method
dvisc	0.0000235	Paxs	904.82	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=U355839&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355839&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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