

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

<b>Inchi:</b>	InChI=1S/C22H40O4/c1-4-6-8-13-16-20(3)26-22(24)18-15-12-10-9-11-14-17-21(23)25-1
<b>InchiKey:</b>	RVZAEKITVVSSHL-DTQAZKPQSA-N
<b>Formula:</b>	C22H40O4
<b>SMILES:</b>	CCCCC=CC(C)OC(=O)CCCCCCCC(=O)OCCCC
<b>Mol. weight [g/mol]:</b>	368.55

## Physical Properties

Property code	Value	Unit	Source
gf	-255.70	kJ/mol	Joback Method
hf	-875.07	kJ/mol	Joback Method
hfus	54.99	kJ/mol	Joback Method
hvap	82.45	kJ/mol	Joback Method
log10ws	-6.72		Crippen Method
logp	6.129		Crippen Method
mcvol	331.420	ml/mol	McGowan Method
pc	990.13	kPa	Joback Method
rinpola	2473.00		NIST Webbook
tb	859.06	K	Joback Method
tc	1052.46	K	Joback Method
tf	461.94	K	Joback Method
vc	1.290	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1066.29	J/molxK	859.06	Joback Method
cpg	1148.14	J/molxK	1020.23	Joback Method
cpg	1133.90	J/molxK	987.99	Joback Method
cpg	1118.63	J/molxK	955.76	Joback Method
cpg	1102.30	J/molxK	923.53	Joback Method
cpg	1084.86	J/molxK	891.29	Joback Method
cpg	1161.37	J/molxK	1052.46	Joback Method
dvisc	0.0000317	Paxs	859.06	Joback Method
dvisc	0.0000430	Paxs	792.87	Joback Method

dvisc	0.0000617	Paxs	726.69	Joback Method
dvisc	0.0000950	Paxs	660.50	Joback Method
dvisc	0.0001611	Paxs	594.31	Joback Method
dvisc	0.0003119	Paxs	528.13	Joback Method
dvisc	0.0007296	Paxs	461.94	Joback Method

## Sources

<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.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=U355836&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355836&amp;Units=SI</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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