

# Sebacic acid, cis-non-3-enyl octyl ester

<b>Inchi:</b>	InChI=1S/C27H50O4/c1-3-5-7-9-13-17-21-25-31-27(29)23-19-15-12-11-14-18-22-26(28)
<b>InchiKey:</b>	AKEVBNGNJNFQRG-LGMDPLHJSA-N
<b>Formula:</b>	C27H50O4
<b>SMILES:</b>	CCCCC=CCCOC(=O)CCCCCCCC(=O)OCCCCCCC
<b>Mol. weight [g/mol]:</b>	438.68

## Physical Properties

Property code	Value	Unit	Source
gf	-211.16	kJ/mol	Joback Method
hf	-972.99	kJ/mol	Joback Method
hfus	71.46	kJ/mol	Joback Method
hvap	93.97	kJ/mol	Joback Method
log10ws	-8.70		Crippen Method
logp	8.081		Crippen Method
mvol	401.870	ml/mol	McGowan Method
pc	744.07	kPa	Joback Method
rinpol	3067.00		NIST Webbook
rinpol	3067.00		NIST Webbook
tb	973.90	K	Joback Method
tc	1201.27	K	Joback Method
tf	533.29	K	Joback Method
vc	1.575	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1381.80	J/molxK	973.90	Joback Method
cpg	1473.28	J/molxK	1163.38	Joback Method
cpg	1457.97	J/molxK	1125.48	Joback Method
cpg	1441.24	J/molxK	1087.59	Joback Method
cpg	1423.02	J/molxK	1049.69	Joback Method
cpg	1403.23	J/molxK	1011.80	Joback Method
cpg	1487.25	J/molxK	1201.27	Joback Method
dvisc	0.0000162	Paxs	973.90	Joback Method

dvisc	0.0000218	Paxs	900.46	Joback Method
dvisc	0.0000310	Paxs	827.03	Joback Method
dvisc	0.0000473	Paxs	753.60	Joback Method
dvisc	0.0000788	Paxs	680.16	Joback Method
dvisc	0.0001486	Paxs	606.72	Joback Method
dvisc	0.0003337	Paxs	533.29	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=U355926&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355926&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.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>

## 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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