

# Sebacic acid, pentyl trans-3-hexenyl ester

<b>Inchi:</b>	InChI=1S/C21H38O4/c1-3-5-7-15-19-25-21(23)17-13-11-9-8-10-12-16-20(22)24-18-14-6
<b>InchiKey:</b>	YDPUFZCPFSPOLQ-FNORWQNLSA-N
<b>Formula:</b>	C21H38O4
<b>SMILES:</b>	CCC=CCCOC(=O)CCCCCCCC(=O)OCCCCC
<b>Mol. weight [g/mol]:</b>	354.52

## Physical Properties

Property code	Value	Unit	Source
gf	-261.68	kJ/mol	Joback Method
hf	-849.15	kJ/mol	Joback Method
hfus	55.92	kJ/mol	Joback Method
hvap	80.61	kJ/mol	Joback Method
log10ws	-6.19		Crippen Method
logp	5.740		Crippen Method
mvol	317.330	ml/mol	McGowan Method
pc	1047.33	kPa	Joback Method
rinpol	2478.00		NIST Webbook
tb	836.62	K	Joback Method
tc	1025.83	K	Joback Method
tf	465.67	K	Joback Method
vc	1.240	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1004.47	J/molxK	836.62	Joback Method
cpg	1022.57	J/molxK	868.16	Joback Method
cpg	1039.63	J/molxK	899.69	Joback Method
cpg	1055.65	J/molxK	931.23	Joback Method
cpg	1070.69	J/molxK	962.76	Joback Method
cpg	1084.75	J/molxK	994.30	Joback Method
cpg	1097.88	J/molxK	1025.83	Joback Method
dvisc	0.0006985	Paxs	465.67	Joback Method
dvisc	0.0003282	Paxs	527.50	Joback Method

dvisc	0.0001807	Paxs	589.32	Joback Method
dvisc	0.0001114	Paxs	651.14	Joback Method
dvisc	0.0000747	Paxs	712.97	Joback Method
dvisc	0.0000534	Paxs	774.80	Joback Method
dvisc	0.0000401	Paxs	836.62	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=U356061&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356061&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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