

# Sebacic acid, di(3-hexyl) ester

<b>Inchi:</b>	InChI=1S/C22H42O4/c1-5-15-19(7-3)25-21(23)17-13-11-9-10-12-14-18-22(24)26-20(8-4
<b>InchiKey:</b>	YLKVHLOJYHDIEU-UHFFFAOYSA-N
<b>Formula:</b>	C22H42O4
<b>SMILES:</b>	CCCC(CC)OC(=O)CCCCCCCCC(=O)OC(CC)CCC
<b>Mol. weight [g/mol]:</b>	370.57

## Physical Properties

Property code	Value	Unit	Source
gf	-338.36	kJ/mol	Joback Method
hf	-997.57	kJ/mol	Joback Method
hfus	51.26	kJ/mol	Joback Method
hvap	82.10	kJ/mol	Joback Method
log10ws	-6.98		Crippen Method
logp	6.351		Crippen Method
mcvol	335.720	ml/mol	McGowan Method
pc	963.27	kPa	Joback Method
rinqol	2392.00		NIST Webbook
tb	854.46	K	Joback Method
tc	1046.57	K	Joback Method
tf	452.02	K	Joback Method
vc	1.304	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1092.98	J/molxK	854.46	Joback Method
cpg	1112.15	J/molxK	886.48	Joback Method
cpg	1130.10	J/molxK	918.50	Joback Method
cpg	1146.85	J/molxK	950.51	Joback Method
cpg	1162.43	J/molxK	982.53	Joback Method
cpg	1176.86	J/molxK	1014.55	Joback Method
cpg	1190.16	J/molxK	1046.57	Joback Method
dvisc	0.0009298	Paxs	452.02	Joback Method
dvisc	0.0003731	Paxs	519.09	Joback Method

dvisc	0.0001845	Paxs	586.17	Joback Method
dvisc	0.0001055	Paxs	653.24	Joback Method
dvisc	0.0000669	Paxs	720.31	Joback Method
dvisc	0.0000458	Paxs	787.39	Joback Method
dvisc	0.0000333	Paxs	854.46	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=U355547&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355547&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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