

# Sebacic acid, hexyl 3-hexyl ester

<b>Inchi:</b>	InChI=1S/C22H42O4/c1-4-7-8-15-19-25-21(23)17-13-11-9-10-12-14-18-22(24)26-20(6-3
<b>InchiKey:</b>	KIRJLCHMMMETGD-UHFFFAOYSA-N
<b>Formula:</b>	C22H42O4
<b>SMILES:</b>	CCCCCOC(=O)CCCCCCCC(=O)OC(CC)CCC
<b>Mol. weight [g/mol]:</b>	370.57

## Physical Properties

Property code	Value	Unit	Source
gf	-335.92	kJ/mol	Joback Method
hf	-992.29	kJ/mol	Joback Method
hfus	54.79	kJ/mol	Joback Method
hvap	82.49	kJ/mol	Joback Method
log10ws	-6.87		Crippen Method
logp	6.353		Crippen Method
mvol	335.720	ml/mol	McGowan Method
pc	958.51	kPa	Joback Method
rinpol	2490.00		NIST Webbook
tb	854.90	K	Joback Method
tc	1046.82	K	Joback Method
tf	467.02	K	Joback Method
vc	1.310	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1092.52	J/molxK	854.90	Joback Method
cpg	1111.68	J/molxK	886.89	Joback Method
cpg	1129.63	J/molxK	918.87	Joback Method
cpg	1146.40	J/molxK	950.86	Joback Method
cpg	1162.01	J/molxK	982.84	Joback Method
cpg	1176.47	J/molxK	1014.83	Joback Method
cpg	1189.83	J/molxK	1046.82	Joback Method
dvisc	0.0007814	Paxs	467.02	Joback Method
dvisc	0.0003435	Paxs	531.67	Joback Method

dvisc	0.0001805	Paxs	596.31	Joback Method
dvisc	0.0001075	Paxs	660.96	Joback Method
dvisc	0.0000703	Paxs	725.61	Joback Method
dvisc	0.0000492	Paxs	790.25	Joback Method
dvisc	0.0000364	Paxs	854.90	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=U355541&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355541&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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