

# Sebacic acid, hexyl 3-methylbut-2-yl ester

<b>Inchi:</b>	InChI=1S/C21H40O4/c1-5-6-7-14-17-24-20(22)15-12-10-8-9-11-13-16-21(23)25-19(4)18
<b>InchiKey:</b>	FGYVQDOQLXTPEQ-UHFFFAOYSA-N
<b>Formula:</b>	C21H40O4
<b>SMILES:</b>	CCCCCOC(=O)CCCCCCCC(=O)OC(C)C(C)C
<b>Mol. weight [g/mol]:</b>	356.54

## Physical Properties

Property code	Value	Unit	Source
gf	-346.78	kJ/mol	Joback Method
hf	-976.93	kJ/mol	Joback Method
hfus	48.67	kJ/mol	Joback Method
hvap	79.88	kJ/mol	Joback Method
log10ws	-6.21		Crippen Method
logp	5.818		Crippen Method
mvol	321.630	ml/mol	McGowan Method
pc	1023.34	kPa	Joback Method
rmpol	2401.00		NIST Webbook
tb	831.58	K	Joback Method
tc	1019.89	K	Joback Method
tf	440.75	K	Joback Method
vc	1.248	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1031.20	J/molxK	831.58	Joback Method
cpg	1049.98	J/molxK	862.97	Joback Method
cpg	1067.62	J/molxK	894.35	Joback Method
cpg	1084.13	J/molxK	925.74	Joback Method
cpg	1099.54	J/molxK	957.12	Joback Method
cpg	1113.87	J/molxK	988.51	Joback Method
cpg	1127.14	J/molxK	1019.89	Joback Method
dvisc	0.0010562	Paxs	440.75	Joback Method
dvisc	0.0004270	Paxs	505.89	Joback Method

dvisc	0.0002123	Paxs	571.03	Joback Method
dvisc	0.0001217	Paxs	636.16	Joback Method
dvisc	0.0000774	Paxs	701.30	Joback Method
dvisc	0.0000532	Paxs	766.44	Joback Method
dvisc	0.0000387	Paxs	831.58	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U355562&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355562&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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