

# Sebacic acid, hexyl 2-methylbutyl ester

<b>Inchi:</b>	InChI=1S/C21H40O4/c1-4-6-7-14-17-24-20(22)15-12-10-8-9-11-13-16-21(23)25-18-19(3)
<b>InchiKey:</b>	HTJDFICRWWHCES-UHFFFAOYSA-N
<b>Formula:</b>	C21H40O4
<b>SMILES:</b>	CCCCCOC(=O)CCCCCCCC(=O)OCC(C)CC
<b>Mol. weight [g/mol]:</b>	356.54

## Physical Properties

Property code	Value	Unit	Source
gf	-344.34	kJ/mol	Joback Method
hf	-971.65	kJ/mol	Joback Method
hfus	52.20	kJ/mol	Joback Method
hvap	80.26	kJ/mol	Joback Method
log10ws	-6.10		Crippen Method
logp	5.820		Crippen Method
mvol	321.630	ml/mol	McGowan Method
pc	1018.13	kPa	Joback Method
rinpol	2483.00		NIST Webbook
tb	832.02	K	Joback Method
tc	1019.80	K	Joback Method
tf	455.75	K	Joback Method
vc	1.254	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1030.73	J/molxK	832.02	Joback Method
cpg	1049.46	J/molxK	863.32	Joback Method
cpg	1067.07	J/molxK	894.61	Joback Method
cpg	1083.56	J/molxK	925.91	Joback Method
cpg	1098.97	J/molxK	957.21	Joback Method
cpg	1113.31	J/molxK	988.51	Joback Method
cpg	1126.61	J/molxK	1019.80	Joback Method
dvisc	0.0008818	Paxs	455.75	Joback Method
dvisc	0.0003912	Paxs	518.46	Joback Method

dvisc	0.0002068	Paxs	581.17	Joback Method
dvisc	0.0001238	Paxs	643.88	Joback Method
dvisc	0.0000812	Paxs	706.60	Joback Method
dvisc	0.0000570	Paxs	769.31	Joback Method
dvisc	0.0000422	Paxs	832.02	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=U354340&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354340&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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