

# Sebacic acid, isobutyl 3-methylbutyl ester

<b>Inchi:</b>	InChI=1S/C19H36O4/c1-16(2)13-14-22-18(20)11-9-7-5-6-8-10-12-19(21)23-15-17(3)4/h1
<b>InchiKey:</b>	MPTACSBEPGLK-UHFFFAOYSA-N
<b>Formula:</b>	C19H36O4
<b>SMILES:</b>	CC(C)CCOC(=O)CCCCCCCCC(=O)OCC(C)C
<b>Mol. weight [g/mol]:</b>	328.49

## Physical Properties

Property code	Value	Unit	Source
gf	-363.62	kJ/mol	Joback Method
hf	-935.65	kJ/mol	Joback Method
hfus	43.49	kJ/mol	Joback Method
hvap	75.42	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	4.896		Crippen Method
mvol	293.450	ml/mol	McGowan Method
pc	1161.66	kPa	Joback Method
rmpol	2208.00		NIST Webbook
tb	785.82	K	Joback Method
tc	968.88	K	Joback Method
tf	418.21	K	Joback Method
vc	1.135	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	909.87	J/molxK	785.82	Joback Method
cpg	927.92	J/molxK	816.33	Joback Method
cpg	944.96	J/molxK	846.84	Joback Method
cpg	961.00	J/molxK	877.35	Joback Method
cpg	976.05	J/molxK	907.86	Joback Method
cpg	990.13	J/molxK	938.37	Joback Method
cpg	1003.26	J/molxK	968.88	Joback Method
dvisc	0.0013492	Paxs	418.21	Joback Method
dvisc	0.0005543	Paxs	479.48	Joback Method

dvisc	0.0002785	Paxs	540.75	Joback Method
dvisc	0.0001610	Paxs	602.01	Joback Method
dvisc	0.0001030	Paxs	663.28	Joback Method
dvisc	0.0000711	Paxs	724.55	Joback Method
dvisc	0.0000520	Paxs	785.82	Joback Method

## Sources

<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=U355366&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355366&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>

## 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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