

# Sebacic acid, 3-methylpentyl propyl ester

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

## Physical Properties

Property code	Value	Unit	Source
gf	-361.18	kJ/mol	Joback Method
hf	-930.37	kJ/mol	Joback Method
hfus	47.02	kJ/mol	Joback Method
hvap	75.81	kJ/mol	Joback Method
log10ws	-5.26		Crippen Method
logp	5.040		Crippen Method
mcvol	293.450	ml/mol	McGowan Method
pc	1155.35	kPa	Joback Method
rinqol	2268.00		NIST Webbook
tb	786.26	K	Joback Method
tc	968.16	K	Joback Method
tf	433.21	K	Joback Method
vc	1.141	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	909.39	J/molxK	786.26	Joback Method
cpg	989.26	J/molxK	937.85	Joback Method
cpg	975.21	J/molxK	907.53	Joback Method
cpg	960.22	J/molxK	877.21	Joback Method
cpg	944.26	J/molxK	846.89	Joback Method
cpg	927.32	J/molxK	816.58	Joback Method
cpg	1002.36	J/molxK	968.16	Joback Method
dvisc	0.0000565	Paxs	786.26	Joback Method
dvisc	0.0000759	Paxs	727.42	Joback Method

dvisc	0.0001075	Paxs	668.58	Joback Method
dvisc	0.0001628	Paxs	609.74	Joback Method
dvisc	0.0002693	Paxs	550.89	Joback Method
dvisc	0.0005025	Paxs	492.05	Joback Method
dvisc	0.0011109	Paxs	433.21	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=U355613&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355613&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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