

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

<b>Inchi:</b>	InChI=1S/C18H34O4/c1-5-14-21-17(19)12-10-8-6-7-9-11-13-18(20)22-16(4)15(2)3/h15-1
<b>InchiKey:</b>	KJWGQDSUPXQFAJ-UHFFFAOYSA-N
<b>Formula:</b>	C18H34O4
<b>SMILES:</b>	CCCOC(=O)CCCCCCCCC(=O)OC(C)C(C)C
<b>Mol. weight [g/mol]:</b>	314.46

## Physical Properties

Property code	Value	Unit	Source
gf	-372.04	kJ/mol	Joback Method
hf	-915.01	kJ/mol	Joback Method
hfus	40.90	kJ/mol	Joback Method
hvap	73.20	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	4.648		Crippen Method
mcvol	279.360	ml/mol	McGowan Method
pc	1241.58	kPa	Joback Method
rinsol	2106.00		NIST Webbook
tb	762.94	K	Joback Method
tc	944.42	K	Joback Method
tf	406.94	K	Joback Method
vc	1.079	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	850.46	J/molxK	762.94	Joback Method
cpg	868.17	J/molxK	793.19	Joback Method
cpg	884.91	J/molxK	823.43	Joback Method
cpg	900.70	J/molxK	853.68	Joback Method
cpg	915.55	J/molxK	883.93	Joback Method
cpg	929.48	J/molxK	914.17	Joback Method
cpg	942.50	J/molxK	944.42	Joback Method
dvisc	0.0015163	Paxs	406.94	Joback Method
dvisc	0.0006283	Paxs	466.27	Joback Method

dvisc	0.0003176	Paxs	525.61	Joback Method
dvisc	0.0001844	Paxs	584.94	Joback Method
dvisc	0.0001183	Paxs	644.27	Joback Method
dvisc	0.0000818	Paxs	703.61	Joback Method
dvisc	0.0000599	Paxs	762.94	Joback Method

## Sources

<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=U355558&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355558&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>

## 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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