

# Succinic acid, nonyl 3-oxobut-2-yl ester

**Inchi:** InChI=1S/C17H30O5/c1-4-5-6-7-8-9-10-13-21-16(19)11-12-17(20)22-15(3)14(2)18/h15H  
**InchiKey:** UHOMHLBNZITWFO-UHFFFAOYSA-N  
**Formula:** C17H30O5  
**SMILES:** CCCCCCCCCOC(=O)CCC(=O)OC(C)C(C)=O  
**Mol. weight [g/mol]:** 314.42

## Physical Properties

Property code	Value	Unit	Source
gf	-506.94	kJ/mol	Joback Method
hf	-1001.67	kJ/mol	Joback Method
hfus	43.44	kJ/mol	Joback Method
hvap	78.11	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.581		Crippen Method
mvol	266.840	ml/mol	McGowan Method
pc	1385.05	kPa	Joback Method
rinpol	2118.00		NIST Webbook
rinpol	2118.00		NIST Webbook
tb	794.37	K	Joback Method
tc	981.67	K	Joback Method
tf	460.60	K	Joback Method
vc	1.036	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	814.28	J/molxK	794.37	Joback Method
cpg	883.78	J/molxK	950.45	Joback Method
cpg	871.76	J/molxK	919.24	Joback Method
cpg	858.81	J/molxK	888.02	Joback Method
cpg	844.92	J/molxK	856.80	Joback Method
cpg	830.08	J/molxK	825.59	Joback Method
cpg	894.88	J/molxK	981.67	Joback Method
dvisc	0.0000717	Paxs	794.37	Joback Method

dvisc	0.0000947	Paxs	738.74	Joback Method
dvisc	0.0001308	Paxs	683.11	Joback Method
dvisc	0.0001914	Paxs	627.49	Joback Method
dvisc	0.0003015	Paxs	571.86	Joback Method
dvisc	0.0005239	Paxs	516.23	Joback Method
dvisc	0.0010403	Paxs	460.60	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U349584&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U349584&amp;Units=SI</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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