

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

<b>Inchi:</b>	InChI=1S/C19H34O5/c1-4-5-6-7-8-9-12-15-23-18(21)13-10-11-14-19(22)24-17(3)16(2)20
<b>InchiKey:</b>	AJGKTYBMOJMFNK-UHFFFAOYSA-N
<b>Formula:</b>	C19H34O5
<b>SMILES:</b>	CCCCCCCCCOC(=O)CCCCC(=O)OC(C)C(C)=O
<b>Mol. weight [g/mol]:</b>	342.47

## Physical Properties

Property code	Value	Unit	Source
gf	-490.10	kJ/mol	Joback Method
hf	-1042.95	kJ/mol	Joback Method
hfus	48.62	kJ/mol	Joback Method
hvap	82.56	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	4.361		Crippen Method
mcvol	295.020	ml/mol	McGowan Method
pc	1206.47	kPa	Joback Method
rinqol	2333.00		NIST Webbook
tb	840.13	K	Joback Method
tc	1031.64	K	Joback Method
tf	483.14	K	Joback Method
vc	1.147	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	932.24	J/molxK	840.13	Joback Method
cpg	948.74	J/molxK	872.05	Joback Method
cpg	964.15	J/molxK	903.97	Joback Method
cpg	978.50	J/molxK	935.88	Joback Method
cpg	991.79	J/molxK	967.80	Joback Method
cpg	1004.05	J/molxK	999.72	Joback Method
cpg	1015.28	J/molxK	1031.64	Joback Method
dvisc	0.0008351	Paxs	483.14	Joback Method
dvisc	0.0004114	Paxs	542.64	Joback Method

dvisc	0.0002331	Paxs	602.14	Joback Method
dvisc	0.0001463	Paxs	661.63	Joback Method
dvisc	0.0000991	Paxs	721.13	Joback Method
dvisc	0.0000713	Paxs	780.63	Joback Method
dvisc	0.0000537	Paxs	840.13	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U353753&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U353753&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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