

# Adipic acid, cis-non-3-enyl propyl ester

<b>Inchi:</b>	InChI=1S/C18H32O4/c1-3-5-6-7-8-9-12-16-22-18(20)14-11-10-13-17(19)21-15-4-2/h8-9H
<b>InchiKey:</b>	FXCKRODYHIEWEO-HJWRWDBZSA-N
<b>Formula:</b>	C18H32O4
<b>SMILES:</b>	CCCCC=CCCOC(=O)CCCC(=O)OCCC
<b>Mol. weight [g/mol]:</b>	312.44

## Physical Properties

Property code	Value	Unit	Source
gf	-286.94	kJ/mol	Joback Method
hf	-787.23	kJ/mol	Joback Method
hfus	48.15	kJ/mol	Joback Method
hvap	73.93	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.570		Crippen Method
mcvol	275.060	ml/mol	McGowan Method
pc	1273.69	kPa	Joback Method
rinqol	2133.00		NIST Webbook
tb	767.98	K	Joback Method
tc	950.09	K	Joback Method
tf	431.86	K	Joback Method
vc	1.071	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	825.20	J/molxK	767.98	Joback Method
cpg	900.81	J/molxK	919.74	Joback Method
cpg	887.40	J/molxK	889.39	Joback Method
cpg	873.15	J/molxK	859.03	Joback Method
cpg	858.05	J/molxK	828.68	Joback Method
cpg	842.07	J/molxK	798.33	Joback Method
cpg	913.41	J/molxK	950.09	Joback Method
dvisc	0.0000613	Paxs	767.98	Joback Method
dvisc	0.0000809	Paxs	711.96	Joback Method

dvisc	0.0001121	Paxs	655.94	Joback Method
dvisc	0.0001651	Paxs	599.92	Joback Method
dvisc	0.0002633	Paxs	543.90	Joback Method
dvisc	0.0004674	Paxs	487.88	Joback Method
dvisc	0.0009629	Paxs	431.86	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=U353989&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U353989&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>
<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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