

# Adipic acid, 3,3-dimethylbut-2-yl hexyl ester

<b>Inchi:</b>	InChI=1S/C18H34O4/c1-6-7-8-11-14-21-16(19)12-9-10-13-17(20)22-15(2)18(3,4)5/h15H
<b>InchiKey:</b>	PJACXVBEPFCDFQ-UHFFFAOYSA-N
<b>Formula:</b>	C18H34O4
<b>SMILES:</b>	CCCCCOC(=O)CCCC(=O)OC(C)C(C)(C)C
<b>Mol. weight [g/mol]:</b>	314.46

## Physical Properties

Property code	Value	Unit	Source
gf	-366.76	kJ/mol	Joback Method
hf	-918.48	kJ/mol	Joback Method
hfus	37.01	kJ/mol	Joback Method
hvap	72.29	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	4.648		Crippen Method
mcvol	279.360	ml/mol	McGowan Method
pc	1251.26	kPa	Joback Method
rinqol	2010.00		NIST Webbook
tb	760.15	K	Joback Method
tc	944.42	K	Joback Method
tf	424.36	K	Joback Method
vc	1.075	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	851.53	J/molxK	760.15	Joback Method
cpg	869.25	J/molxK	790.86	Joback Method
cpg	885.98	J/molxK	821.57	Joback Method
cpg	901.76	J/molxK	852.29	Joback Method
cpg	916.60	J/molxK	883.00	Joback Method
cpg	930.53	J/molxK	913.71	Joback Method
cpg	943.57	J/molxK	944.42	Joback Method
dvisc	0.0012334	Paxs	424.36	Joback Method
dvisc	0.0005382	Paxs	480.32	Joback Method

dvisc	0.0002793	Paxs	536.29	Joback Method
dvisc	0.0001640	Paxs	592.25	Joback Method
dvisc	0.0001056	Paxs	648.22	Joback Method
dvisc	0.0000729	Paxs	704.18	Joback Method
dvisc	0.0000532	Paxs	760.15	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=U353671&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U353671&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>mccvol:</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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