

# Adipic acid, hexyl 3-methylpentyl ester

<b>Inchi:</b>	InChI=1S/C18H34O4/c1-4-6-7-10-14-21-17(19)11-8-9-12-18(20)22-15-13-16(3)5-2/h16H
<b>InchiKey:</b>	QMEBAAAVXAKOEJ-UHFFFAOYSA-N
<b>Formula:</b>	C18H34O4
<b>SMILES:</b>	CCCCCOC(=O)CCCC(=O)OCCC(C)CC
<b>Mol. weight [g/mol]:</b>	314.46

## Physical Properties

Property code	Value	Unit	Source
gf	-369.60	kJ/mol	Joback Method
hf	-909.73	kJ/mol	Joback Method
hfus	44.43	kJ/mol	Joback Method
hvap	73.59	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	4.650		Crippen Method
mcvol	279.360	ml/mol	McGowan Method
pc	1234.61	kPa	Joback Method
rinpola	2112.00		NIST Webbook
tb	763.38	K	Joback Method
tc	943.41	K	Joback Method
tf	421.94	K	Joback Method
vc	1.085	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	849.98	J/molxK	763.38	Joback Method
cpg	928.46	J/molxK	913.41	Joback Method
cpg	914.60	J/molxK	883.40	Joback Method
cpg	899.82	J/molxK	853.40	Joback Method
cpg	884.14	J/molxK	823.39	Joback Method
cpg	867.53	J/molxK	793.39	Joback Method
cpg	941.44	J/molxK	943.41	Joback Method
dvisc	0.0000651	Paxs	763.38	Joback Method
dvisc	0.0000873	Paxs	706.47	Joback Method

dvisc	0.0001232	Paxs	649.57	Joback Method
dvisc	0.0001858	Paxs	592.66	Joback Method
dvisc	0.0003058	Paxs	535.75	Joback Method
dvisc	0.0005664	Paxs	478.85	Joback Method
dvisc	0.0012393	Paxs	421.94	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=U353691&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U353691&amp;Units=SI</a>

## Legend

<b>cp<sub>g</sub>:</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>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>m<sub>cvol</sub>:</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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