

# Adipic acid, isohexyl 2-methylpent-3-yl ester

<b>Inchi:</b>	InChI=1S/C18H34O4/c1-6-16(15(4)5)22-18(20)12-8-7-11-17(19)21-13-9-10-14(2)3/h14-1
<b>InchiKey:</b>	XDQLPYGQZOCXOR-UHFFFAOYSA-N
<b>Formula:</b>	C18H34O4
<b>SMILES:</b>	CCC(OC(=O)CCCCC(=O)OCCCC(C)C)C(C)C
<b>Mol. weight [g/mol]:</b>	314.46

## Physical Properties

Property code	Value	Unit	Source
gf	-374.48	kJ/mol	Joback Method
hf	-920.29	kJ/mol	Joback Method
hfus	37.38	kJ/mol	Joback Method
hvap	72.81	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	4.504		Crippen Method
mcvol	279.360	ml/mol	McGowan Method
pc	1248.61	kPa	Joback Method
rinsol	2002.00		NIST Webbook
tb	762.50	K	Joback Method
tc	945.56	K	Joback Method
tf	391.94	K	Joback Method
vc	1.073	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	850.95	J/molxK	762.50	Joback Method
cpg	868.82	J/molxK	793.01	Joback Method
cpg	885.70	J/molxK	823.52	Joback Method
cpg	901.60	J/molxK	854.03	Joback Method
cpg	916.55	J/molxK	884.54	Joback Method
cpg	930.54	J/molxK	915.05	Joback Method
cpg	943.60	J/molxK	945.56	Joback Method
dvisc	0.0019037	Paxs	391.94	Joback Method
dvisc	0.0007062	Paxs	453.70	Joback Method

dvisc	0.0003322	Paxs	515.46	Joback Method
dvisc	0.0001837	Paxs	577.22	Joback Method
dvisc	0.0001139	Paxs	638.98	Joback Method
dvisc	0.0000768	Paxs	700.74	Joback Method
dvisc	0.0000552	Paxs	762.50	Joback Method

## Sources

<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=U353560&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U353560&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>

## 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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