

# Adipic acid, 3-methylbutyl pentyl ester

<b>Inchi:</b>	InChI=1S/C16H30O4/c1-4-5-8-12-19-15(17)9-6-7-10-16(18)20-13-11-14(2)3/h14H,4-13H
<b>InchiKey:</b>	UFPWFPCFLAFQIX-UHFFFAOYSA-N
<b>Formula:</b>	C16H30O4
<b>SMILES:</b>	CCCCCOC(=O)CCCCC(=O)OCCC(C)C
<b>Mol. weight [g/mol]:</b>	286.41

## Physical Properties

Property code	Value	Unit	Source
gf	-386.44	kJ/mol	Joback Method
hf	-868.45	kJ/mol	Joback Method
hfus	39.25	kJ/mol	Joback Method
hvap	69.13	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	3.870		Crippen Method
mvol	251.180	ml/mol	McGowan Method
pc	1419.71	kPa	Joback Method
rinpol	1924.00		NIST Webbook
rinpol	1924.00		NIST Webbook
tb	717.62	K	Joback Method
tc	895.76	K	Joback Method
tf	399.40	K	Joback Method
vc	0.974	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	734.08	J/molxK	717.62	Joback Method
cpg	809.59	J/molxK	866.07	Joback Method
cpg	796.13	J/molxK	836.38	Joback Method
cpg	781.86	J/molxK	806.69	Joback Method
cpg	766.77	J/molxK	777.00	Joback Method
cpg	750.85	J/molxK	747.31	Joback Method
cpg	822.23	J/molxK	895.76	Joback Method
dvisc	0.0000856	Paxs	717.62	Joback Method

dvisc	0.0001142	Paxs	664.58	Joback Method
dvisc	0.0001602	Paxs	611.55	Joback Method
dvisc	0.0002395	Paxs	558.51	Joback Method
dvisc	0.0003898	Paxs	505.47	Joback Method
dvisc	0.0007109	Paxs	452.44	Joback Method
dvisc	0.0015210	Paxs	399.40	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=U348966&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348966&amp;Units=SI</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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