

# Adipic acid, hexyl pent-4-enyl ester

<b>Inchi:</b>	InChI=1S/C17H30O4/c1-3-5-7-11-15-21-17(19)13-9-8-12-16(18)20-14-10-6-4-2/h4H,2-3,
<b>InchiKey:</b>	GOAGTLJBVXMPKD-UHFFFAOYSA-N
<b>Formula:</b>	C17H30O4
<b>SMILES:</b>	C=CCCCOC(=O)CCCC(=O)OCCCCC
<b>Mol. weight [g/mol]:</b>	298.42

## Physical Properties

Property code	Value	Unit	Source
gf	-287.74	kJ/mol	Joback Method
hf	-758.38	kJ/mol	Joback Method
hfus	44.08	kJ/mol	Joback Method
hvap	71.08	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	4.180		Crippen Method
mcvol	260.970	ml/mol	McGowan Method
pc	1355.63	kPa	Joback Method
rinqol	2045.00		NIST Webbook
tb	737.62	K	Joback Method
tc	916.09	K	Joback Method
tf	423.91	K	Joback Method
vc	1.016	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	765.83	J/molxK	737.62	Joback Method
cpg	782.30	J/molxK	767.36	Joback Method
cpg	797.92	J/molxK	797.11	Joback Method
cpg	812.71	J/molxK	826.85	Joback Method
cpg	826.68	J/molxK	856.60	Joback Method
cpg	839.84	J/molxK	886.34	Joback Method
cpg	852.20	J/molxK	916.09	Joback Method
dvisc	0.0011463	Paxs	423.91	Joback Method
dvisc	0.0005872	Paxs	476.20	Joback Method

dvisc	0.0003434	Paxs	528.48	Joback Method
dvisc	0.0002212	Paxs	580.77	Joback Method
dvisc	0.0001532	Paxs	633.05	Joback Method
dvisc	0.0001122	Paxs	685.34	Joback Method
dvisc	0.0000859	Paxs	737.62	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=U353795&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U353795&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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