

# Adipic acid, hexadecyl pent-4-en-2-yl ester

<b>Inchi:</b>	InChI=1S/C27H50O4/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-20-24-30-26(28)22-18-19-2
<b>InchiKey:</b>	IRYCIXGKQUXYAI-UHFFFAOYSA-N
<b>Formula:</b>	C27H50O4
<b>SMILES:</b>	<chem>C=CCC(C)OC(=O)CCCC(=O)OCCCCCCCCCCCCCCC</chem>
<b>Mol. weight [g/mol]:</b>	438.68

## Physical Properties

Property code	Value	Unit	Source
gf	-205.98	kJ/mol	Joback Method
hf	-970.06	kJ/mol	Joback Method
hfus	66.46	kJ/mol	Joback Method
hvap	92.95	kJ/mol	Joback Method
log10ws	-8.82		Crippen Method
logp	8.079		Crippen Method
mcvol	401.870	ml/mol	McGowan Method
pc	743.26	kPa	Joback Method
rinpola	2949.00		NIST Webbook
tb	965.98	K	Joback Method
tc	1190.59	K	Joback Method
tf	521.61	K	Joback Method
vc	1.571	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1380.03	J/molxK	965.98	Joback Method
cpg	1469.43	J/molxK	1153.16	Joback Method
cpg	1454.73	J/molxK	1115.72	Joback Method
cpg	1438.50	J/molxK	1078.29	Joback Method
cpg	1420.68	J/molxK	1040.85	Joback Method
cpg	1401.21	J/molxK	1003.42	Joback Method
cpg	1482.67	J/molxK	1190.59	Joback Method
dvisc	0.0000182	Paxs	965.98	Joback Method
dvisc	0.0000247	Paxs	891.92	Joback Method

dvisc	0.0000355	Paxs	817.86	Joback Method
dvisc	0.0000547	Paxs	743.80	Joback Method
dvisc	0.0000929	Paxs	669.73	Joback Method
dvisc	0.0001800	Paxs	595.67	Joback Method
dvisc	0.0004208	Paxs	521.61	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=U354131&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354131&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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