

# Adipic acid, pentyl tetradec-11-enyl ester

<b>Inchi:</b>	InChI=1S/C25H46O4/c1-3-5-7-8-9-10-11-12-13-14-15-19-23-29-25(27)21-17-16-20-24(2
<b>InchiKey:</b>	YVDNRHHQSFMONF-FNORWQNLSA-N
<b>Formula:</b>	C25H46O4
<b>SMILES:</b>	CCC=CCCCCCCCCOC(=O)CCCC(=O)OCCCCC
<b>Mol. weight [g/mol]:</b>	410.63

## Physical Properties

Property code	Value	Unit	Source
gf	-228.00	kJ/mol	Joback Method
hf	-931.71	kJ/mol	Joback Method
hfus	66.28	kJ/mol	Joback Method
hvap	89.51	kJ/mol	Joback Method
log10ws	-7.87		Crippen Method
logp	7.300		Crippen Method
mcvol	373.690	ml/mol	McGowan Method
pc	828.59	kPa	Joback Method
rinqol	2827.00		NIST Webbook
tb	928.14	K	Joback Method
tc	1138.56	K	Joback Method
tf	510.75	K	Joback Method
vc	1.464	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1253.80	J/molxK	928.14	Joback Method
cpg	1341.10	J/molxK	1103.49	Joback Method
cpg	1326.20	J/molxK	1068.42	Joback Method
cpg	1310.08	J/molxK	1033.35	Joback Method
cpg	1292.67	J/molxK	998.28	Joback Method
cpg	1273.93	J/molxK	963.21	Joback Method
cpg	1354.81	J/molxK	1138.56	Joback Method
dvisc	0.0000221	Paxs	928.14	Joback Method
dvisc	0.0000297	Paxs	858.58	Joback Method

dvisc	0.0000420	Paxs	789.01	Joback Method
dvisc	0.0000635	Paxs	719.44	Joback Method
dvisc	0.0001049	Paxs	649.88	Joback Method
dvisc	0.0001956	Paxs	580.31	Joback Method
dvisc	0.0004320	Paxs	510.75	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U353785&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U353785&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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