

# Adipic acid, heptadecyl trans-hex-3-enyl ester

**Inchi:** InChI=1S/C29H54O4/c1-3-5-7-9-10-11-12-13-14-15-16-17-18-19-23-27-33-29(31)25-21-  
**InchiKey:** HVGZSWXSJBLGNE-SOFGYWHQSA-N  
**Formula:** C29H54O4  
**SMILES:** CCC=CCCOC(=O)CCCCC(=O)OCCCCCCCCCCCCCCCCCC  
**Mol. weight [g/mol]:** 466.74

## Physical Properties

Property code	Value	Unit	Source
gf	-194.32	kJ/mol	Joback Method
hf	-1014.27	kJ/mol	Joback Method
hfus	76.64	kJ/mol	Joback Method
hvap	98.42	kJ/mol	Joback Method
log10ws	-9.54		Crippen Method
logp	8.861		Crippen Method
mvol	430.050	ml/mol	McGowan Method
pc	671.85	kPa	Joback Method
rinpol	3235.00		NIST Webbook
rinpol	3235.00		NIST Webbook
tb	1019.66	K	Joback Method
tc	1269.19	K	Joback Method
tf	555.83	K	Joback Method
vc	1.688	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1511.50	J/molxK	1019.66	Joback Method
cpg	1534.47	J/molxK	1061.25	Joback Method
cpg	1555.46	J/molxK	1102.84	Joback Method
cpg	1574.59	J/molxK	1144.42	Joback Method
cpg	1591.97	J/molxK	1186.01	Joback Method
cpg	1607.70	J/molxK	1227.60	Joback Method
cpg	1621.89	J/molxK	1269.19	Joback Method
dvisc	0.0002552	Paxs	555.83	Joback Method

dvisc	0.0001119	Paxs	633.13	Joback Method
dvisc	0.0000587	Paxs	710.44	Joback Method
dvisc	0.0000349	Paxs	787.74	Joback Method
dvisc	0.0000228	Paxs	865.05	Joback Method
dvisc	0.0000160	Paxs	942.36	Joback Method
dvisc	0.0000118	Paxs	1019.66	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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=U354021&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354021&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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