

# Adipic acid, heptadecyl 2-propylphenyl ester

<b>Inchi:</b>	InChI=1S/C32H54O4/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-22-28-35-31(33)26-20-21
<b>InchiKey:</b>	MECXJHRLNXXFMLO-UHFFFAOYSA-N
<b>Formula:</b>	C32H54O4
<b>SMILES:</b>	CCCCCCCCCCCCCCCCOC(=O)CCCC(=O)Oc1ccccc1CCC
<b>Mol. weight [g/mol]:</b>	502.77

## Physical Properties

Property code	Value	Unit	Source
gf	-146.50	kJ/mol	Joback Method
hf	-968.35	kJ/mol	Joback Method
hfus	77.86	kJ/mol	Joback Method
hvap	108.08	kJ/mol	Joback Method
log10ws	-10.66		Crippen Method
logp	9.520		Crippen Method
mvol	452.860	ml/mol	McGowan Method
pc	663.57	kPa	Joback Method
rinpol	3598.00		NIST Webbook
rinpol	3598.00		NIST Webbook
tb	1115.80	K	Joback Method
tc	1396.06	K	Joback Method
tf	633.66	K	Joback Method
vc	1.768	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1625.08	J/molxK	1115.80	Joback Method
cpg	1645.08	J/molxK	1162.51	Joback Method
cpg	1662.56	J/molxK	1209.22	Joback Method
cpg	1677.68	J/molxK	1255.93	Joback Method
cpg	1690.58	J/molxK	1302.64	Joback Method
cpg	1701.41	J/molxK	1349.35	Joback Method
cpg	1710.32	J/molxK	1396.06	Joback Method
dvisc	0.0001399	Paxs	633.66	Joback Method

dvisc	0.0000682	Paxs	714.02	Joback Method
dvisc	0.0000385	Paxs	794.37	Joback Method
dvisc	0.0000241	Paxs	874.73	Joback Method
dvisc	0.0000163	Paxs	955.09	Joback Method
dvisc	0.0000118	Paxs	1035.44	Joback Method
dvisc	0.0000089	Paxs	1115.80	Joback Method

## Sources

<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=U353840&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U353840&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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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