

# Adipic acid, hexadecyl 4-methylpent-2-yl ester

**Inchi:** InChI=1S/C28H54O4/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-20-23-31-27(29)21-18-19-2  
**InchiKey:** HPRRSOMZSPBFEO-UHFFFAOYSA-N  
**Formula:** C28H54O4  
**SMILES:** CCCCCCCCCCCCCCCCOC(=O)CCCCC(=O)OC(C)CC(C)C  
**Mol. weight [g/mol]:** 454.73

## Physical Properties

Property code	Value	Unit	Source
gf	-287.84	kJ/mol	Joback Method
hf	-1121.41	kJ/mol	Joback Method
hfus	66.80	kJ/mol	Joback Method
hvap	95.46	kJ/mol	Joback Method
log10ws	-9.14		Crippen Method
logp	8.549		Crippen Method
mvol	420.260	ml/mol	McGowan Method
pc	693.25	kPa	Joback Method
rinpol	2995.00		NIST Webbook
rinpol	2995.00		NIST Webbook
tb	991.74	K	Joback Method
tc	1227.53	K	Joback Method
tf	519.64	K	Joback Method
vc	1.639	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1475.15	J/molxK	991.74	Joback Method
cpg	1497.37	J/molxK	1031.04	Joback Method
cpg	1517.59	J/molxK	1070.34	Joback Method
cpg	1535.87	J/molxK	1109.64	Joback Method
cpg	1552.29	J/molxK	1148.93	Joback Method
cpg	1566.92	J/molxK	1188.23	Joback Method
cpg	1579.83	J/molxK	1227.53	Joback Method
dvisc	0.0004088	Paxs	519.64	Joback Method

dvisc	0.0001579	Paxs	598.32	Joback Method
dvisc	0.0000761	Paxs	677.01	Joback Method
dvisc	0.0000427	Paxs	755.69	Joback Method
dvisc	0.0000267	Paxs	834.37	Joback Method
dvisc	0.0000181	Paxs	913.06	Joback Method
dvisc	0.0000131	Paxs	991.74	Joback Method

## Sources

<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=U353512&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U353512&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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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