

# Pimelic acid, hexyl 2-methylpropyl ester

<b>Inchi:</b>	InChI=1S/C17H32O4/c1-4-5-6-10-13-20-16(18)11-8-7-9-12-17(19)21-14-15(2)3/h15H,4-
<b>InchiKey:</b>	BPNBMFAEAFBFCD-UHFFFAOYSA-N
<b>Formula:</b>	C17H32O4
<b>SMILES:</b>	CCCCCOC(=O)CCCCC(=O)OCC(C)C
<b>Mol. weight [g/mol]:</b>	300.43

## Physical Properties

Property code	Value	Unit	Source
gf	-378.02	kJ/mol	Joback Method
hf	-889.09	kJ/mol	Joback Method
hfus	41.84	kJ/mol	Joback Method
hvap	71.36	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	4.260		Crippen Method
mvol	265.270	ml/mol	McGowan Method
pc	1322.31	kPa	Joback Method
rinpol	2032.00		NIST Webbook
rinpol	2032.00		NIST Webbook
tb	740.50	K	Joback Method
tc	919.30	K	Joback Method
tf	410.67	K	Joback Method
vc	1.030	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	791.52	J/molxK	740.50	Joback Method
cpg	808.68	J/molxK	770.30	Joback Method
cpg	824.95	J/molxK	800.10	Joback Method
cpg	840.35	J/molxK	829.90	Joback Method
cpg	854.88	J/molxK	859.70	Joback Method
cpg	868.56	J/molxK	889.50	Joback Method
cpg	881.39	J/molxK	919.30	Joback Method
dvisc	0.0013763	Paxs	410.67	Joback Method

dvisc	0.0006360	Paxs	465.64	Joback Method
dvisc	0.0003459	Paxs	520.61	Joback Method
dvisc	0.0002113	Paxs	575.59	Joback Method
dvisc	0.0001407	Paxs	630.56	Joback Method
dvisc	0.0001000	Paxs	685.53	Joback Method
dvisc	0.0000748	Paxs	740.50	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.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=U393853&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393853&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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