

# Pimelic acid, 3-methyl-2-pentyl propyl ester

<b>Inchi:</b>	InChI=1S/C16H30O4/c1-5-12-19-15(17)10-8-7-9-11-16(18)20-14(4)13(3)6-2/h13-14H,5-
<b>InchiKey:</b>	KBHBYEXCKRTXGV-UHFFFAOYSA-N
<b>Formula:</b>	C16H30O4
<b>SMILES:</b>	CCCOC(=O)CCCCC(=O)OC(C)C(C)CC
<b>Mol. weight [g/mol]:</b>	286.41

## Physical Properties

Property code	Value	Unit	Source
gf	-388.88	kJ/mol	Joback Method
hf	-873.73	kJ/mol	Joback Method
hfus	35.72	kJ/mol	Joback Method
hvap	68.75	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.868		Crippen Method
mvol	251.180	ml/mol	McGowan Method
pc	1428.30	kPa	Joback Method
rinpol	1879.00		NIST Webbook
rinpol	1879.00		NIST Webbook
tb	717.18	K	Joback Method
tc	897.32	K	Joback Method
tf	384.40	K	Joback Method
vc	0.968	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	734.56	J/molxK	717.18	Joback Method
cpg	751.53	J/molxK	747.20	Joback Method
cpg	767.64	J/molxK	777.23	Joback Method
cpg	782.89	J/molxK	807.25	Joback Method
cpg	797.29	J/molxK	837.27	Joback Method
cpg	810.84	J/molxK	867.29	Joback Method
cpg	823.57	J/molxK	897.32	Joback Method
dvisc	0.0018907	Paxs	384.40	Joback Method

dvisc	0.0007981	Paxs	439.86	Joback Method
dvisc	0.0004087	Paxs	495.33	Joback Method
dvisc	0.0002395	Paxs	550.79	Joback Method
dvisc	0.0001547	Paxs	606.25	Joback Method
dvisc	0.0001076	Paxs	661.72	Joback Method
dvisc	0.0000791	Paxs	717.18	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U406593&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406593&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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