

# Pimelic acid, 4-methyl-2-pentyl 2-propyl ester

<b>Inchi:</b>	InChI=1S/C16H30O4/c1-12(2)11-14(5)20-16(18)10-8-6-7-9-15(17)19-13(3)4/h12-14H,6-
<b>InchiKey:</b>	GODUKMAQBAIDPT-UHFFFAOYSA-N
<b>Formula:</b>	C16H30O4
<b>SMILES:</b>	CC(C)CC(C)OC(=O)CCCCC(=O)OC(C)C
<b>Mol. weight [g/mol]:</b>	286.41

## Physical Properties

Property code	Value	Unit	Source
gf	-391.32	kJ/mol	Joback Method
hf	-879.01	kJ/mol	Joback Method
hfus	32.20	kJ/mol	Joback Method
hvap	68.36	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.866		Crippen Method
mvol	251.180	ml/mol	McGowan Method
pc	1436.98	kPa	Joback Method
rinpol	1766.00		NIST Webbook
rinpol	1766.00		NIST Webbook
tb	716.74	K	Joback Method
tc	899.00	K	Joback Method
tf	369.40	K	Joback Method
vc	0.962	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.04	J/molxK	716.74	Joback Method
cpg	812.14	J/molxK	868.62	Joback Method
cpg	798.48	J/molxK	838.25	Joback Method
cpg	783.94	J/molxK	807.87	Joback Method
cpg	768.53	J/molxK	777.49	Joback Method
cpg	752.23	J/molxK	747.12	Joback Method
cpg	824.95	J/molxK	899.00	Joback Method
dvisc	0.0000731	Paxs	716.74	Joback Method

dvisc	0.0001014	Paxs	658.85	Joback Method
dvisc	0.0001497	Paxs	600.96	Joback Method
dvisc	0.0002403	Paxs	543.07	Joback Method
dvisc	0.0004318	Paxs	485.18	Joback Method
dvisc	0.0009093	Paxs	427.29	Joback Method
dvisc	0.0024183	Paxs	369.40	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=U406557&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406557&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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