

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

<b>Inchi:</b>	InChI=1S/C21H40O4/c1-16(2)13-18(4)25-20(23)12-10-8-9-11-19(22)24-15-17(3)14-21(5)
<b>InchiKey:</b>	ORDLIHMNBKOVLT-UHFFFAOYSA-N
<b>Formula:</b>	C21H40O4
<b>SMILES:</b>	CC(C)CC(C)OC(=O)CCCCC(=O)OCC(C)CC(C)(C)C
<b>Mol. weight [g/mol]:</b>	356.54

## Physical Properties

Property code	Value	Unit	Source
gf	-346.38	kJ/mol	Joback Method
hf	-990.96	kJ/mol	Joback Method
hfus	37.74	kJ/mol	Joback Method
hvap	78.19	kJ/mol	Joback Method
log10ws	-5.72		Crippen Method
logp	5.530		Crippen Method
mvol	321.630	ml/mol	McGowan Method
pc	1041.25	kPa	Joback Method
rinpol	1665.00		NIST Webbook
rinpol	1665.00		NIST Webbook
tb	827.91	K	Joback Method
tc	1019.21	K	Joback Method
tf	428.17	K	Joback Method
vc	1.230	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1032.42	J/molxK	827.91	Joback Method
cpg	1051.28	J/molxK	859.79	Joback Method
cpg	1068.97	J/molxK	891.68	Joback Method
cpg	1085.54	J/molxK	923.56	Joback Method
cpg	1101.01	J/molxK	955.44	Joback Method
cpg	1115.42	J/molxK	987.33	Joback Method
cpg	1128.80	J/molxK	1019.21	Joback Method
dvisc	0.0012756	Paxs	428.17	Joback Method

dvisc	0.0004409	Paxs	494.79	Joback Method
dvisc	0.0001961	Paxs	561.42	Joback Method
dvisc	0.0001036	Paxs	628.04	Joback Method
dvisc	0.0000618	Paxs	694.66	Joback Method
dvisc	0.0000404	Paxs	761.29	Joback Method
dvisc	0.0000283	Paxs	827.91	Joback Method

## Sources

<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=U406471&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406471&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>

## Legend

<b>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>w<sub>s</sub>:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mc<sub>vol</sub>:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rin<sub>pol</sub>:</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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