

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

Inchi:	InChI=1S/C19H36O4/c1-6-10-16(4)14-22-18(20)11-8-7-9-12-19(21)23-17(5)13-15(2)3/h
InchiKey:	QWIZDBGEYROCIU-UHFFFAOYSA-N
Formula:	C19H36O4
SMILES:	CCCC(C)COC(=O)CCCCC(=O)OC(C)CC(C)C
Mol. weight [g/mol]:	328.49

## Physical Properties

Property code	Value	Unit	Source
gf	-366.06	kJ/mol	Joback Method
hf	-940.93	kJ/mol	Joback Method
hfus	39.97	kJ/mol	Joback Method
hvap	75.04	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	4.894		Crippen Method
mcvol	293.450	ml/mol	McGowan Method
pc	1168.02	kPa	Joback Method
rinpol	2074.00		NIST Webbook
rinpol	2074.00		NIST Webbook
tb	785.38	K	Joback Method
tc	969.72	K	Joback Method
tf	403.21	K	Joback Method
vc	1.129	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	910.35	J/molxK	785.38	Joback Method
cpg	928.54	J/molxK	816.10	Joback Method
cpg	945.69	J/molxK	846.83	Joback Method
cpg	961.82	J/molxK	877.55	Joback Method
cpg	976.93	J/molxK	908.28	Joback Method
cpg	991.06	J/molxK	939.00	Joback Method
cpg	1004.20	J/molxK	969.72	Joback Method
dvisc	0.0016792	Paxs	403.21	Joback Method

dvisc	0.0006190	Paxs	466.90	Joback Method
dvisc	0.0002900	Paxs	530.60	Joback Method
dvisc	0.0001598	Paxs	594.29	Joback Method
dvisc	0.0000989	Paxs	657.99	Joback Method
dvisc	0.0000666	Paxs	721.68	Joback Method
dvisc	0.0000478	Paxs	785.38	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U406665&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406665&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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