

# Pimelic acid, 2-methylphenyl pentyl ester

<b>Inchi:</b>	InChI=1S/C19H28O4/c1-3-4-10-15-22-18(20)13-6-5-7-14-19(21)23-17-12-9-8-11-16(17)2
<b>InchiKey:</b>	QAUVAJQYKHNVLZ-UHFFFAOYSA-N
<b>Formula:</b>	C19H28O4
<b>SMILES:</b>	CCCCCOC(=O)CCCCC(=O)Oc1ccccc1C
<b>Mol. weight [g/mol]:</b>	320.42

## Physical Properties

Property code	Value	Unit	Source
gf	-255.96	kJ/mol	Joback Method
hf	-700.03	kJ/mol	Joback Method
hfus	44.19	kJ/mol	Joback Method
hvap	79.14	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	4.584		Crippen Method
mcvol	269.690	ml/mol	McGowan Method
pc	1441.35	kPa	Joback Method
rinsol	2452.00		NIST Webbook
tb	818.36	K	Joback Method
tc	1017.87	K	Joback Method
tf	487.15	K	Joback Method
vc	1.040	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	819.06	J/molxK	818.36	Joback Method
cpg	834.97	J/molxK	851.61	Joback Method
cpg	849.80	J/molxK	884.86	Joback Method
cpg	863.56	J/molxK	918.12	Joback Method
cpg	876.27	J/molxK	951.37	Joback Method
cpg	887.96	J/molxK	984.62	Joback Method
cpg	898.65	J/molxK	1017.87	Joback Method
dvisc	0.0006541	Paxs	487.15	Joback Method
dvisc	0.0003630	Paxs	542.35	Joback Method

dvisc	0.0002246	Paxs	597.55	Joback Method
dvisc	0.0001507	Paxs	652.75	Joback Method
dvisc	0.0001077	Paxs	707.96	Joback Method
dvisc	0.0000807	Paxs	763.16	Joback Method
dvisc	0.0000629	Paxs	818.36	Joback Method

## Sources

<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=U416487&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U416487&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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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