

# Pimelic acid, butyl 2-propyl ester

<b>Inchi:</b>	InChI=1S/C14H26O4/c1-4-5-11-17-13(15)9-7-6-8-10-14(16)18-12(2)3/h12H,4-11H2,1-3H
<b>InchiKey:</b>	VTHVDRPEYWZMBD-UHFFFAOYSA-N
<b>Formula:</b>	C14H26O4
<b>SMILES:</b>	CCCCOC(=O)CCCCC(=O)OC(C)C
<b>Mol. weight [g/mol]:</b>	258.35

## Physical Properties

Property code	Value	Unit	Source
gf	-403.28	kJ/mol	Joback Method
hf	-827.17	kJ/mol	Joback Method
hfus	34.07	kJ/mol	Joback Method
hvap	64.68	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	3.232		Crippen Method
mcvol	223.000	ml/mol	McGowan Method
pc	1649.77	kPa	Joback Method
rinpol	1708.00		NIST Webbook
rinpol	1708.00		NIST Webbook
tb	671.86	K	Joback Method
tc	850.20	K	Joback Method
tf	376.86	K	Joback Method
vc	0.862	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	622.64	J/molxK	671.86	Joback Method
cpg	638.53	J/molxK	701.58	Joback Method
cpg	653.66	J/molxK	731.31	Joback Method
cpg	668.05	J/molxK	761.03	Joback Method
cpg	681.70	J/molxK	790.75	Joback Method
cpg	694.61	J/molxK	820.48	Joback Method
cpg	706.79	J/molxK	850.20	Joback Method
dvisc	0.0018269	Paxs	376.86	Joback Method

dvisc	0.0008752	Paxs	426.03	Joback Method
dvisc	0.0004883	Paxs	475.19	Joback Method
dvisc	0.0003039	Paxs	524.36	Joback Method
dvisc	0.0002052	Paxs	573.53	Joback Method
dvisc	0.0001474	Paxs	622.69	Joback Method
dvisc	0.0001111	Paxs	671.86	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=U406556&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406556&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>

## Legend

<b>cp<sub>g</sub>:</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>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</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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