

# Pimelic acid, butyl hexyl ester

<b>Inchi:</b>	InChI=1S/C17H32O4/c1-3-5-7-11-15-21-17(19)13-10-8-9-12-16(18)20-14-6-4-2/h3-15H2
<b>InchiKey:</b>	YBJRFLQZQCKWLV-UHFFFAOYSA-N
<b>Formula:</b>	C17H32O4
<b>SMILES:</b>	CCCCCOC(=O)CCCCC(=O)OCCCC
<b>Mol. weight [g/mol]:</b>	300.43

## Physical Properties

Property code	Value	Unit	Source
gf	-375.58	kJ/mol	Joback Method
hf	-883.81	kJ/mol	Joback Method
hfus	45.36	kJ/mol	Joback Method
hvap	71.75	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	4.404		Crippen Method
mvol	265.270	ml/mol	McGowan Method
pc	1314.65	kPa	Joback Method
rinpol	1604.00		NIST Webbook
rinpol	1604.00		NIST Webbook
tb	740.94	K	Joback Method
tc	918.14	K	Joback Method
tf	425.67	K	Joback Method
vc	1.036	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	791.03	J/molxK	740.94	Joback Method
cpg	808.03	J/molxK	770.47	Joback Method
cpg	824.15	J/molxK	800.01	Joback Method
cpg	839.43	J/molxK	829.54	Joback Method
cpg	853.86	J/molxK	859.07	Joback Method
cpg	867.46	J/molxK	888.60	Joback Method
cpg	880.23	J/molxK	918.14	Joback Method
dvisc	0.0011435	Paxs	425.67	Joback Method

dvisc	0.0005773	Paxs	478.21	Joback Method
dvisc	0.0003337	Paxs	530.76	Joback Method
dvisc	0.0002129	Paxs	583.31	Joback Method
dvisc	0.0001463	Paxs	635.85	Joback Method
dvisc	0.0001065	Paxs	688.39	Joback Method
dvisc	0.0000811	Paxs	740.94	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U406434&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406434&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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