

# Pimelic acid, hexadecyl 3-methylbutyl ester

<b>Inchi:</b>	InChI=1S/C28H54O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-20-24-31-27(29)21-18-17-19
<b>InchiKey:</b>	PSVZZMIUJAETMN-UHFFFAOYSA-N
<b>Formula:</b>	C28H54O4
<b>SMILES:</b>	CCCCCCCCCCCCCCCCOC(=O)CCCCC(=O)OCCC(C)C
<b>Mol. weight [g/mol]:</b>	454.73

## Physical Properties

Property code	Value	Unit	Source
gf	-285.40	kJ/mol	Joback Method
hf	-1116.13	kJ/mol	Joback Method
hfus	70.33	kJ/mol	Joback Method
hvap	95.85	kJ/mol	Joback Method
log10ws	-9.03		Crippen Method
logp	8.551		Crippen Method
mvol	420.260	ml/mol	McGowan Method
pc	690.34	kPa	Joback Method
rinpol	3133.00		NIST Webbook
rinpol	3133.00		NIST Webbook
tb	992.18	K	Joback Method
tc	1230.25	K	Joback Method
tf	534.64	K	Joback Method
vc	1.645	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1474.86	J/molxK	992.18	Joback Method
cpg	1567.75	J/molxK	1190.58	Joback Method
cpg	1552.94	J/molxK	1150.90	Joback Method
cpg	1536.31	J/molxK	1111.22	Joback Method
cpg	1517.80	J/molxK	1071.54	Joback Method
cpg	1497.34	J/molxK	1031.86	Joback Method
cpg	1580.84	J/molxK	1230.25	Joback Method
dvisc	0.0000144	Paxs	992.18	Joback Method

dvisc	0.0000196	Paxs	915.92	Joback Method
dvisc	0.0000284	Paxs	839.67	Joback Method
dvisc	0.0000442	Paxs	763.41	Joback Method
dvisc	0.0000759	Paxs	687.15	Joback Method
dvisc	0.0001491	Paxs	610.90	Joback Method
dvisc	0.0003555	Paxs	534.64	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=U393784&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393784&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>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>m<sub>cvol</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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