

# Pimelic acid, octyl 2,4,4-trimethylpentyl ester

<b>Inchi:</b>	InChI=1S/C23H44O4/c1-6-7-8-9-10-14-17-26-21(24)15-12-11-13-16-22(25)27-19-20(2)1
<b>InchiKey:</b>	KGSIQIORKDKRLY-UHFFFAOYSA-N
<b>Formula:</b>	C23H44O4
<b>SMILES:</b>	CCCCCCCCOC(=O)CCCCC(=O)OCC(C)CC(C)(C)C
<b>Mol. weight [g/mol]:</b>	384.59

## Physical Properties

Property code	Value	Unit	Source
gf	-324.66	kJ/mol	Joback Method
hf	-1021.68	kJ/mol	Joback Method
hfus	49.96	kJ/mol	Joback Method
hvap	83.42	kJ/mol	Joback Method
log10ws	-6.69		Crippen Method
logp	6.456		Crippen Method
mvol	349.810	ml/mol	McGowan Method
pc	914.39	kPa	Joback Method
rinpol	1836.00		NIST Webbook
rinpol	1836.00		NIST Webbook
tb	874.55	K	Joback Method
tc	1070.98	K	Joback Method
tf	480.71	K	Joback Method
vc	1.355	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1155.24	J/molxK	874.55	Joback Method
cpg	1240.21	J/molxK	1038.24	Joback Method
cpg	1225.54	J/molxK	1005.50	Joback Method
cpg	1209.75	J/molxK	972.76	Joback Method
cpg	1192.79	J/molxK	940.03	Joback Method
cpg	1174.64	J/molxK	907.29	Joback Method
cpg	1253.82	J/molxK	1070.98	Joback Method
dvisc	0.0000245	Paxs	874.55	Joback Method

dvisc	0.0000339	Paxs	808.91	Joback Method
dvisc	0.0000496	Paxs	743.27	Joback Method
dvisc	0.0000781	Paxs	677.63	Joback Method
dvisc	0.0001358	Paxs	611.99	Joback Method
dvisc	0.0002695	Paxs	546.35	Joback Method
dvisc	0.0006448	Paxs	480.71	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U406476&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406476&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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