

# Pimelic acid, 3,7-dimethyloctyl isobutyl ester

<b>Inchi:</b>	InChI=1S/C21H40O4/c1-17(2)10-9-11-19(5)14-15-24-20(22)12-7-6-8-13-21(23)25-16-18
<b>InchiKey:</b>	VWLXWZBRUIAIKG-UHFFFAOYSA-N
<b>Formula:</b>	C21H40O4
<b>SMILES:</b>	CC(C)CCCC(C)CCOC(=O)CCCCC(=O)OCC(C)C
<b>Mol. weight [g/mol]:</b>	356.54

## Physical Properties

Property code	Value	Unit	Source
gf	-349.22	kJ/mol	Joback Method
hf	-982.21	kJ/mol	Joback Method
hfus	45.15	kJ/mol	Joback Method
hvap	79.49	kJ/mol	Joback Method
log10ws	-5.61		Crippen Method
logp	5.532		Crippen Method
mvol	321.630	ml/mol	McGowan Method
pc	1028.60	kPa	Joback Method
rinpol	2324.00		NIST Webbook
rinpol	2324.00		NIST Webbook
tb	831.14	K	Joback Method
tc	1020.11	K	Joback Method
tf	425.75	K	Joback Method
vc	1.242	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1031.67	J/molxK	831.14	Joback Method
cpg	1050.51	J/molxK	862.64	Joback Method
cpg	1068.19	J/molxK	894.13	Joback Method
cpg	1084.74	J/molxK	925.63	Joback Method
cpg	1100.16	J/molxK	957.12	Joback Method
cpg	1114.48	J/molxK	988.62	Joback Method
cpg	1127.72	J/molxK	1020.11	Joback Method
dvisc	0.0012935	Paxs	425.75	Joback Method

dvisc	0.0004714	Paxs	493.32	Joback Method
dvisc	0.0002191	Paxs	560.88	Joback Method
dvisc	0.0001201	Paxs	628.44	Joback Method
dvisc	0.0000739	Paxs	696.01	Joback Method
dvisc	0.0000496	Paxs	763.58	Joback Method
dvisc	0.0000355	Paxs	831.14	Joback Method

## Sources

<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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=U393736&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393736&amp;Units=SI</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>mccvol:</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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