

# Pimelic acid, 5-methoxy-3-methylpent-2-yl octyl ester

Inchi:	InChI=1S/C22H42O5/c1-5-6-7-8-9-13-17-26-21(23)14-11-10-12-15-22(24)27-20(3)19(2)
InchiKey:	UEJXCFRGHFDMMM-UHFFFAOYSA-N
Formula:	C22H42O5
SMILES:	CCCCCCCCOC(=O)CCCCC(=O)OC(C)C(C)CCOC
Mol. weight [g/mol]:	386.57

## Physical Properties

Property code	Value	Unit	Source
gf	-443.36	kJ/mol	Joback Method
hf	-1129.79	kJ/mol	Joback Method
hfus	52.45	kJ/mol	Joback Method
hvap	84.51	kJ/mol	Joback Method
log10ws	-5.71		Crippen Method
logp	5.445		Crippen Method
mcvol	341.590	ml/mol	McGowan Method
pc	953.19	kPa	Joback Method
rinpol	2551.00		NIST Webbook
rinpol	2551.00		NIST Webbook
tb	876.88	K	Joback Method
tc	1073.55	K	Joback Method
tf	474.25	K	Joback Method
vc	1.321	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1125.01	J/molxK	876.88	Joback Method
cpg	1143.87	J/molxK	909.66	Joback Method
cpg	1161.39	J/molxK	942.44	Joback Method
cpg	1177.58	J/molxK	975.22	Joback Method
cpg	1192.45	J/molxK	1008.00	Joback Method
cpg	1206.02	J/molxK	1040.78	Joback Method
cpg	1218.30	J/molxK	1073.55	Joback Method
dvisc	0.0006124	Paxs	474.25	Joback Method

dvisc	0.0002574	Paxs	541.36	Joback Method
dvisc	0.0001310	Paxs	608.46	Joback Method
dvisc	0.0000762	Paxs	675.57	Joback Method
dvisc	0.0000489	Paxs	742.67	Joback Method
dvisc	0.0000338	Paxs	809.78	Joback Method
dvisc	0.0000247	Paxs	876.88	Joback Method

## Sources

<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=U406721&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406721&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>

## 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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