

# Pimelic acid, 3-(2-methoxyethyl)heptyl undecyl ester

**Inchi:** InChI=1S/C28H54O5/c1-4-6-8-9-10-11-12-13-17-23-32-27(29)19-15-14-16-20-28(30)33-34  
**InchiKey:** BBYYIPGXDVFCOJ-UHFFFAOYSA-N  
**Formula:** C28H54O5  
**SMILES:** CCCCCCCCCCOC(=O)CCCCCC(=O)OCCC(CCCC)CCOC  
**Mol. weight [g/mol]:** 470.73

## Physical Properties

Property code	Value	Unit	Source
gf	-390.40	kJ/mol	Joback Method
hf	-1248.35	kJ/mol	Joback Method
hfus	71.52	kJ/mol	Joback Method
hvap	98.26	kJ/mol	Joback Method
log10ws	-8.11		Crippen Method
logp	7.787		Crippen Method
mvol	426.130	ml/mol	McGowan Method
pc	684.21	kPa	Joback Method
rinpol	3152.00		NIST Webbook
rinpol	3152.00		NIST Webbook
tb	1014.60	K	Joback Method
tc	1263.85	K	Joback Method
tf	556.87	K	Joback Method
vc	1.663	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1506.22	J/molxK	1014.60	Joback Method
cpg	1528.11	J/molxK	1056.14	Joback Method
cpg	1547.60	J/molxK	1097.68	Joback Method
cpg	1564.77	J/molxK	1139.22	Joback Method
cpg	1579.67	J/molxK	1180.76	Joback Method
cpg	1592.37	J/molxK	1222.30	Joback Method
cpg	1602.91	J/molxK	1263.85	Joback Method
dvisc	0.0002359	Paxs	556.87	Joback Method

dvisc	0.0001027	Paxs	633.16	Joback Method
dvisc	0.0000535	Paxs	709.45	Joback Method
dvisc	0.0000316	Paxs	785.73	Joback Method
dvisc	0.0000205	Paxs	862.02	Joback Method
dvisc	0.0000143	Paxs	938.31	Joback Method
dvisc	0.0000105	Paxs	1014.60	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=U406790&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406790&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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