

# Pimelic acid, heptyl 2-(2-methoxyethyl)hexyl ester

Inchi:	InChI=1S/C23H44O5/c1-4-6-8-9-13-18-27-22(24)15-11-10-12-16-23(25)28-20-21(14-7-5
InchiKey:	SIWCZIWKKBXSCU-UHFFFAOYSA-N
Formula:	C23H44O5
SMILES:	CCCCCCCOC(=O)CCCCC(=O)OCC(CCCC)CCOC
Mol. weight [g/mol]:	400.59

## Physical Properties

Property code	Value	Unit	Source
gf	-432.50	kJ/mol	Joback Method
hf	-1145.15	kJ/mol	Joback Method
hfus	58.56	kJ/mol	Joback Method
hvap	87.13	kJ/mol	Joback Method
log10ws	-6.02		Crippen Method
logp	5.837		Crippen Method
mvol	355.680	ml/mol	McGowan Method
pc	894.80	kPa	Joback Method
rinpol	2649.00		NIST Webbook
rinpol	2649.00		NIST Webbook
tb	900.20	K	Joback Method
tc	1102.87	K	Joback Method
tf	500.52	K	Joback Method
vc	1.383	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1187.09	J/molxK	900.20	Joback Method
cpg	1206.41	J/molxK	933.98	Joback Method
cpg	1224.28	J/molxK	967.76	Joback Method
cpg	1240.71	J/molxK	1001.53	Joback Method
cpg	1255.73	J/molxK	1035.31	Joback Method
cpg	1269.34	J/molxK	1069.09	Joback Method
cpg	1281.58	J/molxK	1102.87	Joback Method
dvisc	0.0004611	Paxs	500.52	Joback Method

dvisc	0.0002090	Paxs	567.13	Joback Method
dvisc	0.0001118	Paxs	633.75	Joback Method
dvisc	0.0000674	Paxs	700.36	Joback Method
dvisc	0.0000444	Paxs	766.97	Joback Method
dvisc	0.0000312	Paxs	833.59	Joback Method
dvisc	0.0000231	Paxs	900.20	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=U406746&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406746&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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