

# Pimelic acid, ethyl heptyl ester

<b>Inchi:</b>	InChI=1S/C16H30O4/c1-3-5-6-7-11-14-20-16(18)13-10-8-9-12-15(17)19-4-2/h3-14H2,1-2
<b>InchiKey:</b>	RIBCXKPRBCAGBU-UHFFFAOYSA-N
<b>Formula:</b>	C16H30O4
<b>SMILES:</b>	CCCCCCCOC(=O)CCCCC(=O)OCC
<b>Mol. weight [g/mol]:</b>	286.41

## Physical Properties

Property code	Value	Unit	Source
gf	-384.00	kJ/mol	Joback Method
hf	-863.17	kJ/mol	Joback Method
hfus	42.77	kJ/mol	Joback Method
hvap	69.52	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	4.014		Crippen Method
mvol	251.180	ml/mol	McGowan Method
pc	1411.18	kPa	Joback Method
rinpol	1555.00		NIST Webbook
rinpol	1555.00		NIST Webbook
tb	718.06	K	Joback Method
tc	894.33	K	Joback Method
tf	414.40	K	Joback Method
vc	0.980	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	733.60	J/molxK	718.06	Joback Method
cpg	750.17	J/molxK	747.44	Joback Method
cpg	765.92	J/molxK	776.82	Joback Method
cpg	780.87	J/molxK	806.19	Joback Method
cpg	795.02	J/molxK	835.57	Joback Method
cpg	808.37	J/molxK	864.95	Joback Method
cpg	820.95	J/molxK	894.33	Joback Method
dvisc	0.0012551	Paxs	414.40	Joback Method

dvisc	0.0006418	Paxs	465.01	Joback Method
dvisc	0.0003744	Paxs	515.62	Joback Method
dvisc	0.0002405	Paxs	566.23	Joback Method
dvisc	0.0001661	Paxs	616.84	Joback Method
dvisc	0.0001214	Paxs	667.45	Joback Method
dvisc	0.0000927	Paxs	718.06	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.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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U406507&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406507&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>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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