

# Pimelic acid, hexadecyl hexyl ester

<b>Inchi:</b>	InChI=1S/C29H56O4/c1-3-5-7-9-10-11-12-13-14-15-16-17-18-23-27-33-29(31)25-21-19-
<b>InchiKey:</b>	ZRPGNEPJRKMGIT-UHFFFAOYSA-N
<b>Formula:</b>	C29H56O4
<b>SMILES:</b>	CCCCCCCCCCCCCCCCOC(=O)CCCCC(=O)OCCCCC
<b>Mol. weight [g/mol]:</b>	468.75

## Physical Properties

Property code	Value	Unit	Source
gf	-274.54	kJ/mol	Joback Method
hf	-1131.49	kJ/mol	Joback Method
hfus	76.44	kJ/mol	Joback Method
hvap	98.46	kJ/mol	Joback Method
log10ws	-9.69		Crippen Method
logp	9.085		Crippen Method
mvol	434.350	ml/mol	McGowan Method
pc	654.10	kPa	Joback Method
rinpol	3250.00		NIST Webbook
rinpol	3250.00		NIST Webbook
tb	1015.50	K	Joback Method
tc	1268.62	K	Joback Method
tf	560.91	K	Joback Method
vc	1.708	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1539.74	J/molxK	1015.50	Joback Method
cpg	1635.54	J/molxK	1226.44	Joback Method
cpg	1620.57	J/molxK	1184.25	Joback Method
cpg	1603.59	J/molxK	1142.06	Joback Method
cpg	1584.52	J/molxK	1099.87	Joback Method
cpg	1563.27	J/molxK	1057.69	Joback Method
cpg	1648.61	J/molxK	1268.62	Joback Method
dvisc	0.0000134	Paxs	1015.50	Joback Method

dvisc	0.0000181	Paxs	939.73	Joback Method
dvisc	0.0000258	Paxs	863.97	Joback Method
dvisc	0.0000393	Paxs	788.20	Joback Method
dvisc	0.0000654	Paxs	712.44	Joback Method
dvisc	0.0001230	Paxs	636.67	Joback Method
dvisc	0.0002741	Paxs	560.91	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U406551&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406551&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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