

# Pimelic acid, hexadecyl 2-methylpentyl ester

<b>Inchi:</b>	InChI=1S/C29H56O4/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-21-25-32-28(30)23-19-18-2
<b>InchiKey:</b>	ZNRLKBMFGNHIBT-UHFFFAOYSA-N
<b>Formula:</b>	C29H56O4
<b>SMILES:</b>	CCCCCCCCCCCCCCCCOC(=O)CCCCC(=O)OCC(C)CCC
<b>Mol. weight [g/mol]:</b>	468.75

## Physical Properties

Property code	Value	Unit	Source
gf	-276.98	kJ/mol	Joback Method
hf	-1136.77	kJ/mol	Joback Method
hfus	72.92	kJ/mol	Joback Method
hvap	98.07	kJ/mol	Joback Method
log10ws	-9.45		Crippen Method
logp	8.941		Crippen Method
mvol	434.350	ml/mol	McGowan Method
pc	656.79	kPa	Joback Method
rinpol	3207.00		NIST Webbook
rinpol	3207.00		NIST Webbook
tb	1015.06	K	Joback Method
tc	1265.21	K	Joback Method
tf	545.91	K	Joback Method
vc	1.702	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1539.99	J/molxK	1015.06	Joback Method
cpg	1563.19	J/molxK	1056.75	Joback Method
cpg	1584.14	J/molxK	1098.44	Joback Method
cpg	1602.93	J/molxK	1140.13	Joback Method
cpg	1619.67	J/molxK	1181.83	Joback Method
cpg	1634.42	J/molxK	1223.52	Joback Method
cpg	1647.29	J/molxK	1265.21	Joback Method
dvisc	0.0003091	Paxs	545.91	Joback Method

dvisc	0.0001288	Paxs	624.10	Joback Method
dvisc	0.0000652	Paxs	702.29	Joback Method
dvisc	0.0000378	Paxs	780.49	Joback Method
dvisc	0.0000242	Paxs	858.68	Joback Method
dvisc	0.0000167	Paxs	936.87	Joback Method
dvisc	0.0000122	Paxs	1015.06	Joback Method

## Sources

<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=U406677&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406677&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>

## 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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