

# Pimelic acid, tetradecyl pentyl ester

<b>Inchi:</b>	InChI=1S/C26H50O4/c1-3-5-7-8-9-10-11-12-13-14-15-20-24-30-26(28)22-18-16-17-21-2
<b>InchiKey:</b>	SAROXFKUWORNM-UHFFFAOYSA-N
<b>Formula:</b>	C26H50O4
<b>SMILES:</b>	CCCCCCCCCCCCCOC(=O)CCCCC(=O)OCCCCC
<b>Mol. weight [g/mol]:</b>	426.67

## Physical Properties

Property code	Value	Unit	Source
gf	-299.80	kJ/mol	Joback Method
hf	-1069.57	kJ/mol	Joback Method
hfus	68.67	kJ/mol	Joback Method
hvap	91.78	kJ/mol	Joback Method
log10ws	-8.43		Crippen Method
logp	7.915		Crippen Method
mvol	392.080	ml/mol	McGowan Method
pc	762.26	kPa	Joback Method
rinpol	2890.00		NIST Webbook
rinpol	2890.00		NIST Webbook
tb	946.86	K	Joback Method
tc	1166.44	K	Joback Method
tf	527.10	K	Joback Method
vc	1.540	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1345.23	J/molxK	946.86	Joback Method
cpg	1435.85	J/molxK	1129.84	Joback Method
cpg	1420.89	J/molxK	1093.25	Joback Method
cpg	1404.40	J/molxK	1056.65	Joback Method
cpg	1386.33	J/molxK	1020.05	Joback Method
cpg	1366.62	J/molxK	983.46	Joback Method
cpg	1449.33	J/molxK	1166.44	Joback Method
dvisc	0.0000216	Paxs	946.86	Joback Method

dvisc	0.0000290	Paxs	876.90	Joback Method
dvisc	0.0000410	Paxs	806.94	Joback Method
dvisc	0.0000618	Paxs	736.98	Joback Method
dvisc	0.0001016	Paxs	667.02	Joback Method
dvisc	0.0001878	Paxs	597.06	Joback Method
dvisc	0.0004085	Paxs	527.10	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=U393819&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393819&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>cp<sub>g</sub>:</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>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>m<sub>cvol</sub>:</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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