

# Pimelic acid, 2-methylbutyl tetradecyl ester

<b>Inchi:</b>	InChI=1S/C26H50O4/c1-4-6-7-8-9-10-11-12-13-14-15-19-22-29-25(27)20-17-16-18-21-2
<b>InchiKey:</b>	BUIVRSFPRVGOPF-UHFFFAOYSA-N
<b>Formula:</b>	C26H50O4
<b>SMILES:</b>	CCCCCCCCCCCCCOC(=O)CCCCC(=O)OCC(C)CC
<b>Mol. weight [g/mol]:</b>	426.67

## Physical Properties

Property code	Value	Unit	Source
gf	-302.24	kJ/mol	Joback Method
hf	-1074.85	kJ/mol	Joback Method
hfus	65.15	kJ/mol	Joback Method
hvap	91.39	kJ/mol	Joback Method
log10ws	-8.19		Crippen Method
logp	7.771		Crippen Method
mvol	392.080	ml/mol	McGowan Method
pc	765.64	kPa	Joback Method
rinpol	2920.00		NIST Webbook
rinpol	2920.00		NIST Webbook
tb	946.42	K	Joback Method
tc	1164.49	K	Joback Method
tf	512.10	K	Joback Method
vc	1.534	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1345.59	J/molxK	946.42	Joback Method
cpg	1435.40	J/molxK	1128.14	Joback Method
cpg	1420.58	J/molxK	1091.80	Joback Method
cpg	1404.25	J/molxK	1055.45	Joback Method
cpg	1386.34	J/molxK	1019.11	Joback Method
cpg	1366.80	J/molxK	982.76	Joback Method
cpg	1448.73	J/molxK	1164.49	Joback Method
dvisc	0.0000197	Paxs	946.42	Joback Method

dvisc	0.0000268	Paxs	874.03	Joback Method
dvisc	0.0000387	Paxs	801.65	Joback Method
dvisc	0.0000599	Paxs	729.26	Joback Method
dvisc	0.0001021	Paxs	656.87	Joback Method
dvisc	0.0001988	Paxs	584.49	Joback Method
dvisc	0.0004671	Paxs	512.10	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=U406656&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406656&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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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