

# Pimelic acid, decyl 2,4,4-trimethylpentyl ester

<b>Inchi:</b>	InChI=1S/C25H48O4/c1-6-7-8-9-10-11-12-16-19-28-23(26)17-14-13-15-18-24(27)29-21-
<b>InchiKey:</b>	FYEHTNFCQRDBBW-UHFFFAOYSA-N
<b>Formula:</b>	C25H48O4
<b>SMILES:</b>	CCCCCCCCCOC(=O)CCCCC(=O)OCC(C)CC(C)(C)C
<b>Mol. weight [g/mol]:</b>	412.65

## Physical Properties

Property code	Value	Unit	Source
gf	-307.82	kJ/mol	Joback Method
hf	-1062.96	kJ/mol	Joback Method
hfus	55.14	kJ/mol	Joback Method
hvap	87.87	kJ/mol	Joback Method
log10ws	-7.53		Crippen Method
logp	7.236		Crippen Method
mvol	377.990	ml/mol	McGowan Method
pc	816.79	kPa	Joback Method
rinpol	1940.00		NIST Webbook
rinpol	1940.00		NIST Webbook
tb	920.31	K	Joback Method
tc	1127.45	K	Joback Method
tf	503.25	K	Joback Method
vc	1.466	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1281.45	J/molxK	920.31	Joback Method
cpg	1301.73	J/molxK	954.83	Joback Method
cpg	1320.61	J/molxK	989.36	Joback Method
cpg	1338.12	J/molxK	1023.88	Joback Method
cpg	1354.33	J/molxK	1058.41	Joback Method
cpg	1369.31	J/molxK	1092.93	Joback Method
cpg	1383.09	J/molxK	1127.45	Joback Method
dvisc	0.0004880	Paxs	503.25	Joback Method

dvisc	0.0002009	Paxs	572.76	Joback Method
dvisc	0.0001003	Paxs	642.27	Joback Method
dvisc	0.0000573	Paxs	711.78	Joback Method
dvisc	0.0000362	Paxs	781.29	Joback Method
dvisc	0.0000246	Paxs	850.80	Joback Method
dvisc	0.0000178	Paxs	920.31	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=U406478&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406478&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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