

# Pimelic acid, butyl tridecyl ester

<b>Inchi:</b>	InChI=1S/C24H46O4/c1-3-5-7-8-9-10-11-12-13-14-18-22-28-24(26)20-17-15-16-19-23(2
<b>InchiKey:</b>	JKZJROHLZCWIRZ-UHFFFAOYSA-N
<b>Formula:</b>	C24H46O4
<b>SMILES:</b>	CCCCCCCCCCCCOC(=O)CCCCC(=O)OCCCC
<b>Mol. weight [g/mol]:</b>	398.62

## Physical Properties

Property code	Value	Unit	Source
gf	-316.64	kJ/mol	Joback Method
hf	-1028.29	kJ/mol	Joback Method
hfus	63.49	kJ/mol	Joback Method
hvap	87.33	kJ/mol	Joback Method
log10ws	-7.59		Crippen Method
logp	7.134		Crippen Method
mvol	363.900	ml/mol	McGowan Method
pc	849.99	kPa	Joback Method
rinpol	2752.00		NIST Webbook
rinpol	2752.00		NIST Webbook
tb	901.10	K	Joback Method
tc	1104.70	K	Joback Method
tf	504.56	K	Joback Method
vc	1.427	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1217.58	J/molxK	901.10	Joback Method
cpg	1237.78	J/molxK	935.03	Joback Method
cpg	1256.57	J/molxK	968.97	Joback Method
cpg	1273.99	J/molxK	1002.90	Joback Method
cpg	1290.07	J/molxK	1036.83	Joback Method
cpg	1304.84	J/molxK	1070.77	Joback Method
cpg	1318.35	J/molxK	1104.70	Joback Method
dvisc	0.0005261	Paxs	504.56	Joback Method

dvisc	0.0002463	Paxs	570.65	Joback Method
dvisc	0.0001350	Paxs	636.74	Joback Method
dvisc	0.0000828	Paxs	702.83	Joback Method
dvisc	0.0000553	Paxs	768.92	Joback Method
dvisc	0.0000393	Paxs	835.01	Joback Method
dvisc	0.0000294	Paxs	901.10	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=U406540&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406540&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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