

# Pimelic acid, 2,6-dichlorophenyl undecyl ester

<b>Inchi:</b>	InChI=1S/C24H36Cl2O4/c1-2-3-4-5-6-7-8-9-13-19-29-22(27)17-11-10-12-18-23(28)30-24
<b>InchiKey:</b>	RYNORBLVAQZMNQ-UHFFFAOYSA-N
<b>Formula:</b>	C24H36Cl2O4
<b>SMILES:</b>	CCCCCCCCCOC(=O)CCCCC(=O)Oc1c(Cl)cccc1Cl
<b>Mol. weight [g/mol]:</b>	459.45

## Physical Properties

Property code	Value	Unit	Source
gf	-247.35	kJ/mol	Joback Method
hf	-846.18	kJ/mol	Joback Method
hfus	65.15	kJ/mol	Joback Method
hvap	99.70	kJ/mol	Joback Method
log10ws	-8.72		Crippen Method
logp	7.923		Crippen Method
mvol	364.620	ml/mol	McGowan Method
pc	974.73	kPa	Joback Method
rinpol	3287.00		NIST Webbook
rinpol	3287.00		NIST Webbook
tb	1012.60	K	Joback Method
tc	1239.97	K	Joback Method
tf	615.86	K	Joback Method
vc	1.417	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1169.66	J/molxK	1012.60	Joback Method
cpg	1184.22	J/molxK	1050.50	Joback Method
cpg	1197.29	J/molxK	1088.39	Joback Method
cpg	1208.93	J/molxK	1126.29	Joback Method
cpg	1219.16	J/molxK	1164.18	Joback Method
cpg	1228.05	J/molxK	1202.08	Joback Method
cpg	1235.63	J/molxK	1239.97	Joback Method
dvisc	0.0002177	Paxs	615.86	Joback Method

dvisc	0.0001239	Paxs	681.98	Joback Method
dvisc	0.0000779	Paxs	748.11	Joback Method
dvisc	0.0000528	Paxs	814.23	Joback Method
dvisc	0.0000380	Paxs	880.35	Joback Method
dvisc	0.0000286	Paxs	946.48	Joback Method
dvisc	0.0000223	Paxs	1012.60	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=U416664&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U416664&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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