

# Pimelic acid, 4-chlorophenyl pentadecyl ester

<b>Inchi:</b>	InChI=1S/C28H45ClO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-17-24-32-27(30)18-15-14-16-19
<b>InchiKey:</b>	CFHOKGCFZIDBHM-UHFFFAOYSA-N
<b>Formula:</b>	C28H45ClO4
<b>SMILES:</b>	CCCCCCCCCCCCCCCCOC(=O)CCCCC(=O)Oc1ccc(Cl)cc1
<b>Mol. weight [g/mol]:</b>	481.11

## Physical Properties

Property code	Value	Unit	Source
gf	-192.11	kJ/mol	Joback Method
hf	-901.53	kJ/mol	Joback Method
hfus	71.70	kJ/mol	Joback Method
hvap	103.56	kJ/mol	Joback Method
log10ws	-9.70		Crippen Method
logp	8.830		Crippen Method
mvol	408.740	ml/mol	McGowan Method
pc	800.24	kPa	Joback Method
rinpol	3509.00		NIST Webbook
rinpol	3509.00		NIST Webbook
tb	1061.71	K	Joback Method
tc	1308.18	K	Joback Method
tf	618.50	K	Joback Method
vc	1.593	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1394.96	J/molxK	1061.71	Joback Method
cpg	1462.66	J/molxK	1267.10	Joback Method
cpg	1452.50	J/molxK	1226.02	Joback Method
cpg	1440.73	J/molxK	1184.94	Joback Method
cpg	1427.27	J/molxK	1143.87	Joback Method
cpg	1412.04	J/molxK	1102.79	Joback Method
cpg	1471.32	J/molxK	1308.18	Joback Method
dvisc	0.0000139	Paxs	1061.71	Joback Method

dvisc	0.0000182	Paxs	987.84	Joback Method
dvisc	0.0000250	Paxs	913.97	Joback Method
dvisc	0.0000361	Paxs	840.11	Joback Method
dvisc	0.0000561	Paxs	766.24	Joback Method
dvisc	0.0000957	Paxs	692.37	Joback Method
dvisc	0.0001855	Paxs	618.50	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=U393841&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393841&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>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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