

# Pimelic acid, 3-chlorophenyl ethyl ester

<b>Inchi:</b>	InChI=1S/C15H19ClO4/c1-2-19-14(17)9-4-3-5-10-15(18)20-13-8-6-7-12(16)11-13/h6-8,1
<b>InchiKey:</b>	WVJLVPOFWUCHB-UHFFFAOYSA-N
<b>Formula:</b>	C15H19ClO4
<b>SMILES:</b>	CCOC(=O)CCCCC(=O)Oc1cccc(Cl)c1
<b>Mol. weight [g/mol]:</b>	298.76

## Physical Properties

Property code	Value	Unit	Source
gf	-301.57	kJ/mol	Joback Method
hf	-633.21	kJ/mol	Joback Method
hfus	38.03	kJ/mol	Joback Method
hvap	74.62	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	3.759		Crippen Method
mvol	225.570	ml/mol	McGowan Method
pc	1911.91	kPa	Joback Method
rinpol	2255.00		NIST Webbook
rinpol	2255.00		NIST Webbook
tb	764.27	K	Joback Method
tc	971.48	K	Joback Method
tf	471.99	K	Joback Method
vc	0.865	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	620.06	J/molxK	764.27	Joback Method
cpg	633.75	J/molxK	798.81	Joback Method
cpg	646.48	J/molxK	833.34	Joback Method
cpg	658.28	J/molxK	867.88	Joback Method
cpg	669.14	J/molxK	902.41	Joback Method
cpg	679.09	J/molxK	936.95	Joback Method
cpg	688.14	J/molxK	971.48	Joback Method
dvisc	0.0007853	Paxs	471.99	Joback Method

dvisc	0.0004679	Paxs	520.70	Joback Method
dvisc	0.0003046	Paxs	569.42	Joback Method
dvisc	0.0002121	Paxs	618.13	Joback Method
dvisc	0.0001558	Paxs	666.84	Joback Method
dvisc	0.0001193	Paxs	715.56	Joback Method
dvisc	0.0000945	Paxs	764.27	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=U416667&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U416667&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.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>

## 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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