

# Pimelic acid, 4-chloro-3-methylphenyl hexyl ester

Inchi:	InChI=1S/C20H29ClO4/c1-3-4-5-9-14-24-19(22)10-7-6-8-11-20(23)25-17-12-13-18(21)16
InchiKey:	JTWJDPPCJGCPJA-UHFFFAOYSA-N
Formula:	C20H29ClO4
SMILES:	CCCCCOC(=O)CCCCC(=O)Oc1ccc(Cl)c(C)c1
Mol. weight [g/mol]:	368.89

## Physical Properties

Property code	Value	Unit	Source
gf	-269.10	kJ/mol	Joback Method
hf	-747.88	kJ/mol	Joback Method
hfus	50.59	kJ/mol	Joback Method
hvap	86.41	kJ/mol	Joback Method
log10ws	-6.41		Crippen Method
logp	5.628		Crippen Method
mvol	296.020	ml/mol	McGowan Method
pc	1292.07	kPa	Joback Method
rinpol	2766.00		NIST Webbook
rinpol	2766.00		NIST Webbook
tb	883.65	K	Joback Method
tc	1089.89	K	Joback Method
tf	540.86	K	Joback Method
vc	1.145	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	904.12	J/molxK	883.65	Joback Method
cpg	967.13	J/molxK	1055.52	Joback Method
cpg	956.77	J/molxK	1021.14	Joback Method
cpg	945.31	J/molxK	986.77	Joback Method
cpg	932.72	J/molxK	952.40	Joback Method
cpg	919.00	J/molxK	918.02	Joback Method
cpg	976.41	J/molxK	1089.89	Joback Method
dvisc	0.0000480	Paxs	883.65	Joback Method

dvisc	0.0000609	Paxs	826.52	Joback Method
dvisc	0.0000799	Paxs	769.39	Joback Method
dvisc	0.0001097	Paxs	712.25	Joback Method
dvisc	0.0001590	Paxs	655.12	Joback Method
dvisc	0.0002474	Paxs	597.99	Joback Method
dvisc	0.0004227	Paxs	540.86	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=U416686&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U416686&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>

## 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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