

# Pimelic acid, 4-chlorobenzyl hexyl ester

<b>Inchi:</b>	InChI=1S/C20H29ClO4/c1-2-3-4-8-15-24-19(22)9-6-5-7-10-20(23)25-16-17-11-13-18(21)
<b>InchiKey:</b>	NYVUEBVYIJYAIN-UHFFFAOYSA-N
<b>Formula:</b>	C20H29ClO4
<b>SMILES:</b>	CCCCCOC(=O)CCCCC(=O)OCc1ccc(Cl)cc1
<b>Mol. weight [g/mol]:</b>	368.89

## Physical Properties

Property code	Value	Unit	Source
gf	-259.47	kJ/mol	Joback Method
hf	-736.41	kJ/mol	Joback Method
hfus	50.98	kJ/mol	Joback Method
hvap	85.75	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	5.457		Crippen Method
mcvol	296.020	ml/mol	McGowan Method
pc	1306.12	kPa	Joback Method
rinpol	2655.00		NIST Webbook
rinpol	2655.00		NIST Webbook
tb	878.67	K	Joback Method
tc	1084.02	K	Joback Method
tf	528.34	K	Joback Method
vc	1.145	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	904.96	J/molxK	878.67	Joback Method
cpg	968.55	J/molxK	1049.80	Joback Method
cpg	958.03	J/molxK	1015.57	Joback Method
cpg	946.44	J/molxK	981.35	Joback Method
cpg	933.75	J/molxK	947.12	Joback Method
cpg	919.93	J/molxK	912.90	Joback Method
cpg	978.02	J/molxK	1084.02	Joback Method
dvisc	0.0000473	Paxs	878.67	Joback Method

dvisc	0.0000607	Paxs	820.28	Joback Method
dvisc	0.0000809	Paxs	761.89	Joback Method
dvisc	0.0001132	Paxs	703.50	Joback Method
dvisc	0.0001684	Paxs	645.12	Joback Method
dvisc	0.0002709	Paxs	586.73	Joback Method
dvisc	0.0004842	Paxs	528.34	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=U406797&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406797&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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