

# Pimelic acid, 3,5-dichlorobenzyl octyl ester

<b>Inchi:</b>	InChI=1S/C22H32Cl2O4/c1-2-3-4-5-6-10-13-27-21(25)11-8-7-9-12-22(26)28-17-18-14-19
<b>InchiKey:</b>	MZNXZZEPHREHF-UHFFFAOYSA-N
<b>Formula:</b>	C22H32Cl2O4
<b>SMILES:</b>	CCCCCCCCOC(=O)CCCCC(=O)OCc1cc(Cl)cc(Cl)c1
<b>Mol. weight [g/mol]:</b>	431.39

## Physical Properties

Property code	Value	Unit	Source
gf	-264.19	kJ/mol	Joback Method
hf	-804.90	kJ/mol	Joback Method
hfus	59.97	kJ/mol	Joback Method
hvap	95.25	kJ/mol	Joback Method
log10ws	-7.72		Crippen Method
logp	6.891		Crippen Method
mvol	336.440	ml/mol	McGowan Method
pc	1103.01	kPa	Joback Method
rinpol	2996.00		NIST Webbook
rinpol	2996.00		NIST Webbook
tb	966.84	K	Joback Method
tc	1184.56	K	Joback Method
tf	593.32	K	Joback Method
vc	1.306	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1048.35	J/molxK	966.84	Joback Method
cpg	1062.47	J/molxK	1003.13	Joback Method
cpg	1075.27	J/molxK	1039.41	Joback Method
cpg	1086.79	J/molxK	1075.70	Joback Method
cpg	1097.05	J/molxK	1111.99	Joback Method
cpg	1106.10	J/molxK	1148.27	Joback Method
cpg	1113.96	J/molxK	1184.56	Joback Method
dvisc	0.0002763	Paxs	593.32	Joback Method

dvisc	0.0001606	Paxs	655.57	Joback Method
dvisc	0.0001025	Paxs	717.83	Joback Method
dvisc	0.0000703	Paxs	780.08	Joback Method
dvisc	0.0000510	Paxs	842.33	Joback Method
dvisc	0.0000386	Paxs	904.59	Joback Method
dvisc	0.0000304	Paxs	966.84	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U406689&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406689&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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