

# Diglycolic acid, 4-chloro-2-methylphenyl pentyl ester

<b>Inchi:</b>	InChI=1S/C16H21ClO5/c1-3-4-5-8-21-15(18)10-20-11-16(19)22-14-7-6-13(17)9-12(14)2
<b>InchiKey:</b>	PNTZAOZMYIUXNZ-UHFFFAOYSA-N
<b>Formula:</b>	C16H21ClO5
<b>SMILES:</b>	CCCCCOC(=O)COCC(=O)Oc1ccc(Cl)cc1C
<b>Mol. weight [g/mol]:</b>	328.79

## Physical Properties

Property code	Value	Unit	Source
gf	-407.78	kJ/mol	Joback Method
hf	-797.54	kJ/mol	Joback Method
hfus	41.42	kJ/mol	Joback Method
hvap	79.92	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.304		Crippen Method
mvol	245.530	ml/mol	McGowan Method
pc	1714.61	kPa	Joback Method
rinpol	2825.00		NIST Webbook
rinpol	2825.00		NIST Webbook
tb	814.55	K	Joback Method
tc	1020.52	K	Joback Method
tf	518.01	K	Joback Method
vc	0.939	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	701.40	J/molxK	814.55	Joback Method
cpg	714.92	J/molxK	848.88	Joback Method
cpg	727.39	J/molxK	883.21	Joback Method
cpg	738.82	J/molxK	917.53	Joback Method
cpg	749.20	J/molxK	951.86	Joback Method
cpg	758.53	J/molxK	986.19	Joback Method
cpg	766.80	J/molxK	1020.52	Joback Method
dvisc	0.0004448	Paxs	518.01	Joback Method

dvisc	0.0002788	Paxs	567.43	Joback Method
dvisc	0.0001883	Paxs	616.86	Joback Method
dvisc	0.0001348	Paxs	666.28	Joback Method
dvisc	0.0001011	Paxs	715.70	Joback Method
dvisc	0.0000787	Paxs	765.13	Joback Method
dvisc	0.0000631	Paxs	814.55	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=U382741&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382741&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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