

# Diglycolic acid, 4-chlorophenyl pentyl ester

<b>Inchi:</b>	InChI=1S/C15H19ClO5/c1-2-3-4-9-20-14(17)10-19-11-15(18)21-13-7-5-12(16)6-8-13/h5-
<b>InchiKey:</b>	WCXXZFPOISQDFU-UHFFFAOYSA-N
<b>Formula:</b>	C15H19ClO5
<b>SMILES:</b>	CCCCCOC(=O)COCC(=O)Oc1ccc(Cl)cc1
<b>Mol. weight [g/mol]:</b>	314.76

## Physical Properties

Property code	Value	Unit	Source
gf	-406.57	kJ/mol	Joback Method
hf	-765.43	kJ/mol	Joback Method
hfus	39.22	kJ/mol	Joback Method
hvap	77.03	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	2.995		Crippen Method
mcvol	231.440	ml/mol	McGowan Method
pc	1883.80	kPa	Joback Method
rinsol	2746.00		NIST Webbook
tb	786.69	K	Joback Method
tc	992.98	K	Joback Method
tf	494.22	K	Joback Method
vc	0.882	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	646.85	J/molxK	786.69	Joback Method
cpg	660.17	J/molxK	821.07	Joback Method
cpg	672.50	J/molxK	855.45	Joback Method
cpg	683.83	J/molxK	889.84	Joback Method
cpg	694.17	J/molxK	924.22	Joback Method
cpg	703.51	J/molxK	958.60	Joback Method
cpg	711.86	J/molxK	992.98	Joback Method
dvisc	0.0005613	Paxs	494.22	Joback Method
dvisc	0.0003415	Paxs	542.97	Joback Method

dvisc	0.0002255	Paxs	591.71	Joback Method
dvisc	0.0001586	Paxs	640.45	Joback Method
dvisc	0.0001173	Paxs	689.20	Joback Method
dvisc	0.0000902	Paxs	737.94	Joback Method
dvisc	0.0000717	Paxs	786.69	Joback Method

## Sources

<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=U381779&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381779&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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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