

# Diglycolic acid, 3-chlorophenyl isohexyl ester

**Inchi:** InChI=1S/C16H21ClO5/c1-12(2)5-4-8-21-15(18)10-20-11-16(19)22-14-7-3-6-13(17)9-14/  
**InchiKey:** LUSYYZFNZYJQDR-UHFFFAOYSA-N  
**Formula:** C16H21ClO5  
**SMILES:** CC(C)CCCOC(=O)COCC(=O)Oc1cccc(Cl)c1  
**Mol. weight [g/mol]:** 328.79

## Physical Properties

Property code	Value	Unit	Source
gf	-400.59	kJ/mol	Joback Method
hf	-791.35	kJ/mol	Joback Method
hfus	38.28	kJ/mol	Joback Method
hvap	78.87	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	3.241		Crippen Method
mvol	245.530	ml/mol	McGowan Method
pc	1747.74	kPa	Joback Method
rinpol	2805.00		NIST Webbook
rinpol	2805.00		NIST Webbook
tb	809.13	K	Joback Method
tc	1016.81	K	Joback Method
tf	490.49	K	Joback Method
vc	0.932	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	703.05	J/molxK	809.13	Joback Method
cpg	761.11	J/molxK	982.20	Joback Method
cpg	751.65	J/molxK	947.58	Joback Method
cpg	741.11	J/molxK	912.97	Joback Method
cpg	729.50	J/molxK	878.36	Joback Method
cpg	716.81	J/molxK	843.74	Joback Method
cpg	769.51	J/molxK	1016.81	Joback Method
dvisc	0.0000574	Paxs	809.13	Joback Method

dvisc	0.0000736	Paxs	756.02	Joback Method
dvisc	0.0000981	Paxs	702.92	Joback Method
dvisc	0.0001369	Paxs	649.81	Joback Method
dvisc	0.0002027	Paxs	596.70	Joback Method
dvisc	0.0003241	Paxs	543.60	Joback Method
dvisc	0.0005736	Paxs	490.49	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=U381769&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381769&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>

## 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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