

# Diglycolic acid, hexyl 2,4,6-trichlorophenyl ester

Inchi:	InChI=1S/C16H19Cl3O5/c1-2-3-4-5-6-23-14(20)9-22-10-15(21)24-16-12(18)7-11(17)8-13
InchiKey:	LKHKXTBAYIYREV-UHFFFAOYSA-N
Formula:	C16H19Cl3O5
SMILES:	CCCCCOC(=O)COCC(=O)Oc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]:	397.68

## Physical Properties

Property code	Value	Unit	Source
gf	-441.27	kJ/mol	Joback Method
hf	-840.49	kJ/mol	Joback Method
hfus	49.42	kJ/mol	Joback Method
hvap	89.35	kJ/mol	Joback Method
log10ws	-5.14		Crippen Method
logp	4.692		Crippen Method
mvol	270.010	ml/mol	McGowan Method
pc	1594.89	kPa	Joback Method
rinpol	3134.00		NIST Webbook
rinpol	3134.00		NIST Webbook
tb	894.39	K	Joback Method
tc	1109.85	K	Joback Method
tf	590.37	K	Joback Method
vc	1.036	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	746.29	J/molxK	894.39	Joback Method
cpg	757.32	J/molxK	930.30	Joback Method
cpg	767.22	J/molxK	966.21	Joback Method
cpg	775.97	J/molxK	1002.12	Joback Method
cpg	783.58	J/molxK	1038.03	Joback Method
cpg	790.04	J/molxK	1073.94	Joback Method
cpg	795.34	J/molxK	1109.85	Joback Method
dvisc	0.0002787	Paxs	590.37	Joback Method

dvisc	0.0001848	Paxs	641.04	Joback Method
dvisc	0.0001301	Paxs	691.71	Joback Method
dvisc	0.0000961	Paxs	742.38	Joback Method
dvisc	0.0000738	Paxs	793.05	Joback Method
dvisc	0.0000585	Paxs	843.72	Joback Method
dvisc	0.0000476	Paxs	894.39	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=U382736&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382736&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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