

# Diglycolic acid, 2,3-dichlorophenyl isohexyl ester

Inchi:	InChI=1S/C16H20Cl2O5/c1-11(2)5-4-8-22-14(19)9-21-10-15(20)23-13-7-3-6-12(17)16(18)
InchiKey:	BSJSIFBVBFFULB-UHFFFAOYSA-N
Formula:	C16H20Cl2O5
SMILES:	CC(C)CCCOC(=O)COCC(=O)Oc1cccc(Cl)c1Cl
Mol. weight [g/mol]:	363.23

## Physical Properties

Property code	Value	Unit	Source
gf	-422.15	kJ/mol	Joback Method
hf	-818.56	kJ/mol	Joback Method
hfus	42.09	kJ/mol	Joback Method
hvap	83.91	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	3.895		Crippen Method
mcvol	257.770	ml/mol	McGowan Method
pc	1674.16	kPa	Joback Method
rinpola	3018.00		NIST Webbook
rinpola	3018.00		NIST Webbook
tb	851.54	K	Joback Method
tc	1064.03	K	Joback Method
tf	532.93	K	Joback Method
vc	0.982	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	726.08	J/molxK	851.54	Joback Method
cpg	777.15	J/molxK	1028.62	Joback Method
cpg	769.18	J/molxK	993.20	Joback Method
cpg	760.08	J/molxK	957.79	Joback Method
cpg	749.86	J/molxK	922.37	Joback Method
cpg	738.53	J/molxK	886.96	Joback Method
cpg	784.00	J/molxK	1064.03	Joback Method
dvisc	0.0000501	Paxs	851.54	Joback Method

dvisc	0.0000633	Paxs	798.44	Joback Method
dvisc	0.0000826	Paxs	745.34	Joback Method
dvisc	0.0001123	Paxs	692.24	Joback Method
dvisc	0.0001608	Paxs	639.13	Joback Method
dvisc	0.0002456	Paxs	586.03	Joback Method
dvisc	0.0004081	Paxs	532.93	Joback Method

## Sources

<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=U382092&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382092&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>

## Legend

<b>cp<sub>g</sub>:</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>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>m<sub>cvol</sub>:</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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