

# Diglycolic acid, butyl 2,3-dichlorophenyl ester

<b>Inchi:</b>	InChI=1S/C14H16Cl2O5/c1-2-3-7-20-12(17)8-19-9-13(18)21-11-6-4-5-10(15)14(11)16/h
<b>InchiKey:</b>	DUMAWGVBP GSACG-UHFFFAOYSA-N
<b>Formula:</b>	C14H16Cl2O5
<b>SMILES:</b>	CCCCOC(=O)COCC(=O)Oc1cccc(Cl)c1Cl
<b>Mol. weight [g/mol]:</b>	335.18

## Physical Properties

Property code	Value	Unit	Source
gf	-436.55	kJ/mol	Joback Method
hf	-772.00	kJ/mol	Joback Method
hfus	40.43	kJ/mol	Joback Method
hvap	79.85	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	3.259		Crippen Method
mvol	229.590	ml/mol	McGowan Method
pc	1957.87	kPa	Joback Method
rinpol	2807.00		NIST Webbook
rinpol	2807.00		NIST Webbook
tb	806.22	K	Joback Method
tc	1018.57	K	Joback Method
tf	525.39	K	Joback Method
vc	0.875	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	614.67	J/molxK	806.22	Joback Method
cpg	626.44	J/molxK	841.61	Joback Method
cpg	637.25	J/molxK	877.00	Joback Method
cpg	647.07	J/molxK	912.39	Joback Method
cpg	655.89	J/molxK	947.78	Joback Method
cpg	663.71	J/molxK	983.17	Joback Method
cpg	670.52	J/molxK	1018.57	Joback Method
dvisc	0.0004517	Paxs	525.39	Joback Method

dvisc	0.0002939	Paxs	572.19	Joback Method
dvisc	0.0002041	Paxs	619.00	Joback Method
dvisc	0.0001491	Paxs	665.81	Joback Method
dvisc	0.0001136	Paxs	712.61	Joback Method
dvisc	0.0000895	Paxs	759.41	Joback Method
dvisc	0.0000724	Paxs	806.22	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=U382090&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382090&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>

## 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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