

# Diglycolic acid, 3-methylphenyl propyl ester

<b>Inchi:</b>	InChI=1S/C14H18O5/c1-3-7-18-13(15)9-17-10-14(16)19-12-6-4-5-11(2)8-12/h4-6,8H,3,7
<b>InchiKey:</b>	LGXGZJRSWRFIGQ-UHFFFAOYSA-N
<b>Formula:</b>	C14H18O5
<b>SMILES:</b>	CCCOC(=O)COCC(=O)Oc1cccc(C)c1
<b>Mol. weight [g/mol]:</b>	266.29

## Physical Properties

Property code	Value	Unit	Source
gf	-403.06	kJ/mol	Joback Method
hf	-729.05	kJ/mol	Joback Method
hfus	32.43	kJ/mol	Joback Method
hvap	70.42	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	1.870		Crippen Method
mvol	205.110	ml/mol	McGowan Method
pc	2121.68	kPa	Joback Method
rinpol	2388.00		NIST Webbook
rinpol	2388.00		NIST Webbook
tb	726.38	K	Joback Method
tc	930.82	K	Joback Method
tf	453.03	K	Joback Method
vc	0.777	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	566.63	J/molxK	726.38	Joback Method
cpg	580.70	J/molxK	760.45	Joback Method
cpg	593.86	J/molxK	794.53	Joback Method
cpg	606.11	J/molxK	828.60	Joback Method
cpg	617.43	J/molxK	862.68	Joback Method
cpg	627.82	J/molxK	896.75	Joback Method
cpg	637.28	J/molxK	930.82	Joback Method
dvisc	0.0007156	Paxs	453.03	Joback Method

dvisc	0.0004349	Paxs	498.59	Joback Method
dvisc	0.0002873	Paxs	544.15	Joback Method
dvisc	0.0002023	Paxs	589.71	Joback Method
dvisc	0.0001498	Paxs	635.26	Joback Method
dvisc	0.0001155	Paxs	680.82	Joback Method
dvisc	0.0000920	Paxs	726.38	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=U382098&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382098&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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