

# Diglycolic acid, 2,5-dimethylphenyl ethyl ester

<b>Inchi:</b>	InChI=1S/C14H18O5/c1-4-18-13(15)8-17-9-14(16)19-12-7-10(2)5-6-11(12)3/h5-7H,4,8-9
<b>InchiKey:</b>	QWSITZGPORANLE-UHFFFAOYSA-N
<b>Formula:</b>	C14H18O5
<b>SMILES:</b>	CCOC(=O)COCC(=O)Oc1cc(C)ccc1C
<b>Mol. weight [g/mol]:</b>	266.29

## Physical Properties

Property code	Value	Unit	Source
gf	-412.69	kJ/mol	Joback Method
hf	-740.52	kJ/mol	Joback Method
hfus	32.04	kJ/mol	Joback Method
hvap	71.08	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	1.789		Crippen Method
mcvol	205.110	ml/mol	McGowan Method
pc	2092.66	kPa	Joback Method
rinpola	2344.00		NIST Webbook
rinpola	2344.00		NIST Webbook
tb	731.36	K	Joback Method
tc	936.61	K	Joback Method
tf	465.55	K	Joback Method
vc	0.777	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	565.66	J/molxK	731.36	Joback Method
cpg	579.62	J/molxK	765.57	Joback Method
cpg	592.68	J/molxK	799.78	Joback Method
cpg	604.83	J/molxK	833.99	Joback Method
cpg	616.07	J/molxK	868.19	Joback Method
cpg	626.37	J/molxK	902.40	Joback Method
cpg	635.73	J/molxK	936.61	Joback Method
dvisc	0.0006082	Paxs	465.55	Joback Method

dvisc	0.0003873	Paxs	509.85	Joback Method
dvisc	0.0002651	Paxs	554.15	Joback Method
dvisc	0.0001919	Paxs	598.46	Joback Method
dvisc	0.0001452	Paxs	642.76	Joback Method
dvisc	0.0001140	Paxs	687.06	Joback Method
dvisc	0.0000921	Paxs	731.36	Joback Method

## Sources

<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=U382703&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382703&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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

Latest version available from:

<https://www.chemeo.com/cid/82-483-5/Diglycolic-acid-2-5-dimethylphenyl-ethyl-ester.pdf>

Generated by Cheméo on 2024-04-27 07:17:00.943252374 +0000 UTC m=+16491469.863829695.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.