

# Diglycolic acid, pentyl phenethyl ester

<b>Inchi:</b>	InChI=1S/C17H24O5/c1-2-3-7-11-21-16(18)13-20-14-17(19)22-12-10-15-8-5-4-6-9-15/h
<b>InchiKey:</b>	LTEHSTQGVBWSAM-UHFFFAOYSA-N
<b>Formula:</b>	C17H24O5
<b>SMILES:</b>	CCCCCOC(=O)COCC(=O)OCCc1ccccc1
<b>Mol. weight [g/mol]:</b>	308.37

## Physical Properties

Property code	Value	Unit	Source
gf	-368.17	kJ/mol	Joback Method
hf	-779.50	kJ/mol	Joback Method
hfus	40.59	kJ/mol	Joback Method
hvap	76.43	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.522		Crippen Method
mcvol	247.380	ml/mol	McGowan Method
pc	1674.16	kPa	Joback Method
rinpol	2874.00		NIST Webbook
rinpol	2874.00		NIST Webbook
tb	790.04	K	Joback Method
tc	989.47	K	Joback Method
tf	474.32	K	Joback Method
vc	0.946	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	733.48	J/molxK	790.04	Joback Method
cpg	748.59	J/molxK	823.28	Joback Method
cpg	762.65	J/molxK	856.52	Joback Method
cpg	775.65	J/molxK	889.76	Joback Method
cpg	787.62	J/molxK	922.99	Joback Method
cpg	798.55	J/molxK	956.23	Joback Method
cpg	808.46	J/molxK	989.47	Joback Method
dvisc	0.0006571	Paxs	474.32	Joback Method

dvisc	0.0003642	Paxs	526.94	Joback Method
dvisc	0.0002247	Paxs	579.56	Joback Method
dvisc	0.0001502	Paxs	632.18	Joback Method
dvisc	0.0001068	Paxs	684.80	Joback Method
dvisc	0.0000798	Paxs	737.42	Joback Method
dvisc	0.0000619	Paxs	790.04	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=U382159&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382159&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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