

# Diglycolic acid, 2-pentyl propyl ester

<b>Inchi:</b>	InChI=1S/C12H22O5/c1-4-6-10(3)17-12(14)9-15-8-11(13)16-7-5-2/h10H,4-9H2,1-3H3
<b>InchiKey:</b>	ZHLFFVPKZYPWFY-UHFFFAOYSA-N
<b>Formula:</b>	C12H22O5
<b>SMILES:</b>	CCCOC(=O)COCC(=O)OC(C)CCC
<b>Mol. weight [g/mol]:</b>	246.30

## Physical Properties

Property code	Value	Unit	Source
gf	-525.12	kJ/mol	Joback Method
hf	-918.11	kJ/mol	Joback Method
hfus	30.07	kJ/mol	Joback Method
hvap	62.64	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	1.688		Crippen Method
mcvol	200.690	ml/mol	McGowan Method
pc	1911.91	kPa	Joback Method
rinsol	1927.00		NIST Webbook
tb	648.52	K	Joback Method
tc	828.30	K	Joback Method
tf	376.55	K	Joback Method
vc	0.767	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.76	J/molxK	648.52	Joback Method
cpg	558.41	J/molxK	678.48	Joback Method
cpg	572.40	J/molxK	708.45	Joback Method
cpg	585.72	J/molxK	738.41	Joback Method
cpg	598.37	J/molxK	768.38	Joback Method
cpg	610.34	J/molxK	798.34	Joback Method
cpg	621.62	J/molxK	828.30	Joback Method
dvisc	0.0014862	Paxs	376.55	Joback Method
dvisc	0.0007629	Paxs	421.88	Joback Method

dvisc	0.0004458	Paxs	467.21	Joback Method
dvisc	0.0002864	Paxs	512.53	Joback Method
dvisc	0.0001977	Paxs	557.86	Joback Method
dvisc	0.0001443	Paxs	603.19	Joback Method
dvisc	0.0001101	Paxs	648.52	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=U382332&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382332&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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