

# Diglycolic acid, ethyl neopentyl ester

<b>Inchi:</b>	InChI=1S/C11H20O5/c1-5-15-9(12)6-14-7-10(13)16-8-11(2,3)4/h5-8H2,1-4H3
<b>InchiKey:</b>	NAPVEGFHCKMZQK-UHFFFAOYSA-N
<b>Formula:</b>	C11H20O5
<b>SMILES:</b>	CCOC(=O)COCC(=O)OCC(C)(C)C
<b>Mol. weight [g/mol]:</b>	232.27

## Physical Properties

Property code	Value	Unit	Source
gf	-528.26	kJ/mol	Joback Method
hf	-900.94	kJ/mol	Joback Method
hfus	23.59	kJ/mol	Joback Method
hvap	59.51	kJ/mol	Joback Method
log10ws	-1.00		Crippen Method
logp	1.155		Crippen Method
mcvol	186.600	ml/mol	McGowan Method
pc	2104.20	kPa	Joback Method
rinpola	1768.00		NIST Webbook
rinpola	1768.00		NIST Webbook
tb	622.85	K	Joback Method
tc	809.38	K	Joback Method
tf	382.70	K	Joback Method
vc	0.707	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.65	J/molxK	622.85	Joback Method
cpg	559.27	J/molxK	778.29	Joback Method
cpg	547.72	J/molxK	747.20	Joback Method
cpg	535.49	J/molxK	716.11	Joback Method
cpg	522.57	J/molxK	685.03	Joback Method
cpg	508.95	J/molxK	653.94	Joback Method
cpg	570.13	J/molxK	809.38	Joback Method
dvisc	0.0001173	Paxs	622.85	Joback Method

dvisc	0.0001536	Paxs	582.82	Joback Method
dvisc	0.0002093	Paxs	542.80	Joback Method
dvisc	0.0002995	Paxs	502.77	Joback Method
dvisc	0.0004562	Paxs	462.75	Joback Method
dvisc	0.0007524	Paxs	422.73	Joback Method
dvisc	0.0013778	Paxs	382.70	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=U381914&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381914&amp;Units=SI</a>
<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>

## 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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