

# Diglycolic acid, butyl neopentyl ester

<b>Inchi:</b>	InChI=1S/C13H24O5/c1-5-6-7-17-11(14)8-16-9-12(15)18-10-13(2,3)4/h5-10H2,1-4H3
<b>InchiKey:</b>	BDQWQSZWDUICRI-UHFFFAOYSA-N
<b>Formula:</b>	C13H24O5
<b>SMILES:</b>	CCCCOC(=O)COCC(=O)OCC(C)(C)C
<b>Mol. weight [g/mol]:</b>	260.33

## Physical Properties

Property code	Value	Unit	Source
gf	-511.42	kJ/mol	Joback Method
hf	-942.22	kJ/mol	Joback Method
hfus	28.77	kJ/mol	Joback Method
hvap	63.96	kJ/mol	Joback Method
log10ws	-1.83		Crippen Method
logp	1.936		Crippen Method
mvol	214.780	ml/mol	McGowan Method
pc	1777.34	kPa	Joback Method
rinpol	2028.00		NIST Webbook
rinpol	2028.00		NIST Webbook
tb	668.61	K	Joback Method
tc	852.22	K	Joback Method
tf	405.24	K	Joback Method
vc	0.819	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.16	J/molxK	668.61	Joback Method
cpg	668.26	J/molxK	821.62	Joback Method
cpg	655.98	J/molxK	791.02	Joback Method
cpg	642.93	J/molxK	760.42	Joback Method
cpg	629.11	J/molxK	729.81	Joback Method
cpg	614.53	J/molxK	699.21	Joback Method
cpg	679.79	J/molxK	852.22	Joback Method
dvisc	0.0000894	Paxs	668.61	Joback Method

dvisc	0.0001180	Paxs	624.72	Joback Method
dvisc	0.0001622	Paxs	580.82	Joback Method
dvisc	0.0002350	Paxs	536.92	Joback Method
dvisc	0.0003637	Paxs	493.03	Joback Method
dvisc	0.0006130	Paxs	449.13	Joback Method
dvisc	0.0011570	Paxs	405.24	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=U381916&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381916&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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