

# Diglycolic acid, butyl 3-methylbutyl ester

<b>Inchi:</b>	InChI=1S/C13H24O5/c1-4-5-7-17-12(14)9-16-10-13(15)18-8-6-11(2)3/h11H,4-10H2,1-3H
<b>InchiKey:</b>	QWRGQEXIWNFDBS-UHFFFAOYSA-N
<b>Formula:</b>	C13H24O5
<b>SMILES:</b>	CCCCOC(=O)COCC(=O)OCCC(C)C
<b>Mol. weight [g/mol]:</b>	260.33

## Physical Properties

Property code	Value	Unit	Source
gf	-516.70	kJ/mol	Joback Method
hf	-938.75	kJ/mol	Joback Method
hfus	32.66	kJ/mol	Joback Method
hvap	64.87	kJ/mol	Joback Method
log10ws	-1.83		Crippen Method
logp	1.936		Crippen Method
mcvol	214.780	ml/mol	McGowan Method
pc	1760.97	kPa	Joback Method
rinpol	2101.00		NIST Webbook
rinpol	2101.00		NIST Webbook
tb	671.40	K	Joback Method
tc	850.36	K	Joback Method
tf	387.82	K	Joback Method
vc	0.824	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.96	J/molxK	671.40	Joback Method
cpg	612.15	J/molxK	701.23	Joback Method
cpg	626.63	J/molxK	731.05	Joback Method
cpg	640.40	J/molxK	760.88	Joback Method
cpg	653.44	J/molxK	790.71	Joback Method
cpg	665.75	J/molxK	820.53	Joback Method
cpg	677.33	J/molxK	850.36	Joback Method
dvisc	0.0013703	Paxs	387.82	Joback Method

dvisc	0.0006936	Paxs	435.08	Joback Method
dvisc	0.0004012	Paxs	482.35	Joback Method
dvisc	0.0002559	Paxs	529.61	Joback Method
dvisc	0.0001757	Paxs	576.87	Joback Method
dvisc	0.0001277	Paxs	624.14	Joback Method
dvisc	0.0000971	Paxs	671.40	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=U382269&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382269&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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