

# Diglycolic acid, butyl 2-ethylbutyl ester

<b>Inchi:</b>	InChI=1S/C14H26O5/c1-4-7-8-18-13(15)10-17-11-14(16)19-9-12(5-2)6-3/h12H,4-11H2,1
<b>InchiKey:</b>	SXSWOZXWGBIYSK-UHFFFAOYSA-N
<b>Formula:</b>	C14H26O5
<b>SMILES:</b>	CCCCOC(=O)COCC(=O)OCC(CC)CC
<b>Mol. weight [g/mol]:</b>	274.35

## Physical Properties

Property code	Value	Unit	Source
gf	-508.28	kJ/mol	Joback Method
hf	-959.39	kJ/mol	Joback Method
hfus	35.25	kJ/mol	Joback Method
hvap	67.09	kJ/mol	Joback Method
log10ws	-2.25		Crippen Method
logp	2.326		Crippen Method
mcvol	228.870	ml/mol	McGowan Method
pc	1627.22	kPa	Joback Method
rinpol	2254.00		NIST Webbook
rinpol	2254.00		NIST Webbook
tb	694.28	K	Joback Method
tc	872.83	K	Joback Method
tf	399.09	K	Joback Method
vc	0.879	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	651.48	J/molxK	694.28	Joback Method
cpg	667.16	J/molxK	724.04	Joback Method
cpg	682.08	J/molxK	753.80	Joback Method
cpg	696.23	J/molxK	783.56	Joback Method
cpg	709.61	J/molxK	813.32	Joback Method
cpg	722.22	J/molxK	843.08	Joback Method
cpg	734.04	J/molxK	872.83	Joback Method
dvisc	0.0012554	Paxs	399.09	Joback Method

dvisc	0.0006269	Paxs	448.29	Joback Method
dvisc	0.0003592	Paxs	497.49	Joback Method
dvisc	0.0002275	Paxs	546.68	Joback Method
dvisc	0.0001553	Paxs	595.88	Joback Method
dvisc	0.0001124	Paxs	645.08	Joback Method
dvisc	0.0000852	Paxs	694.28	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=U381832&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381832&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>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>w<sub>s</sub>:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mc<sub>vol</sub>:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rin<sub>pol</sub>:</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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