

# Diglycolic acid, di(isobutyl) ester

<b>Inchi:</b>	InChI=1S/C12H22O5/c1-9(2)5-16-11(13)7-15-8-12(14)17-6-10(3)4/h9-10H,5-8H2,1-4H3
<b>InchiKey:</b>	OUAMATOUUTZOLD-UHFFFAOYSA-N
<b>Formula:</b>	C12H22O5
<b>SMILES:</b>	CC(C)COC(=O)COCC(=O)OCC(C)C
<b>Mol. weight [g/mol]:</b>	246.30

## Physical Properties

Property code	Value	Unit	Source
gf	-527.56	kJ/mol	Joback Method
hf	-923.39	kJ/mol	Joback Method
hfus	26.55	kJ/mol	Joback Method
hvap	62.25	kJ/mol	Joback Method
log10ws	-1.17		Crippen Method
logp	1.401		Crippen Method
mcvol	200.690	ml/mol	McGowan Method
pc	1925.36	kPa	Joback Method
rinpola	1915.00		NIST Webbook
rinpola	1915.00		NIST Webbook
tb	648.08	K	Joback Method
tc	830.65	K	Joback Method
tf	361.55	K	Joback Method
vc	0.761	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.21	J/molxK	648.08	Joback Method
cpg	559.13	J/molxK	678.51	Joback Method
cpg	573.35	J/molxK	708.94	Joback Method
cpg	586.88	J/molxK	739.36	Joback Method
cpg	599.71	J/molxK	769.79	Joback Method
cpg	611.82	J/molxK	800.22	Joback Method
cpg	623.21	J/molxK	830.65	Joback Method
dvisc	0.0018669	Paxs	361.55	Joback Method

dvisc	0.0008676	Paxs	409.31	Joback Method
dvisc	0.0004732	Paxs	457.06	Joback Method
dvisc	0.0002895	Paxs	504.81	Joback Method
dvisc	0.0001928	Paxs	552.57	Joback Method
dvisc	0.0001370	Paxs	600.32	Joback Method
dvisc	0.0001023	Paxs	648.08	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U382125&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382125&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>
<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>

## 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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