

# Diglycolic acid, 3-methylbutyl undecyl ester

<b>Inchi:</b>	InChI=1S/C20H38O5/c1-4-5-6-7-8-9-10-11-12-14-24-19(21)16-23-17-20(22)25-15-13-18
<b>InchiKey:</b>	CGSCJBWNMHOIHG-UHFFFAOYSA-N
<b>Formula:</b>	C20H38O5
<b>SMILES:</b>	CCCCCCCCCOC(=O)COCC(=O)OCCC(C)C
<b>Mol. weight [g/mol]:</b>	358.51

## Physical Properties

Property code	Value	Unit	Source
gf	-457.76	kJ/mol	Joback Method
hf	-1083.23	kJ/mol	Joback Method
hfus	50.80	kJ/mol	Joback Method
hvap	80.45	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	4.666		Crippen Method
mcvol	313.410	ml/mol	McGowan Method
pc	1071.46	kPa	Joback Method
rinpol	2964.00		NIST Webbook
rinpol	2964.00		NIST Webbook
tb	831.56	K	Joback Method
tc	1019.41	K	Joback Method
tf	466.71	K	Joback Method
vc	1.216	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1001.32	J/molxK	831.56	Joback Method
cpg	1080.36	J/molxK	988.10	Joback Method
cpg	1066.81	J/molxK	956.79	Joback Method
cpg	1052.14	J/molxK	925.48	Joback Method
cpg	1036.34	J/molxK	894.18	Joback Method
cpg	1019.40	J/molxK	862.87	Joback Method
cpg	1092.80	J/molxK	1019.41	Joback Method
dvisc	0.0000365	Paxs	831.56	Joback Method

dvisc	0.0000489	Paxs	770.75	Joback Method
dvisc	0.0000690	Paxs	709.94	Joback Method
dvisc	0.0001037	Paxs	649.13	Joback Method
dvisc	0.0001697	Paxs	588.33	Joback Method
dvisc	0.0003109	Paxs	527.52	Joback Method
dvisc	0.0006668	Paxs	466.71	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=U382277&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382277&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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