

# Diglycolic acid, 3-methylbutyl tridecyl ester

<b>Inchi:</b>	InChI=1S/C22H42O5/c1-4-5-6-7-8-9-10-11-12-13-14-16-26-21(23)18-25-19-22(24)27-17
<b>InchiKey:</b>	MRHQYGHXKPCHOO-UHFFFAOYSA-N
<b>Formula:</b>	C22H42O5
<b>SMILES:</b>	CCCCCCCCCCCCOC(=O)COCC(=O)OCCC(C)C
<b>Mol. weight [g/mol]:</b>	386.57

## Physical Properties

Property code	Value	Unit	Source
gf	-440.92	kJ/mol	Joback Method
hf	-1124.51	kJ/mol	Joback Method
hfus	55.97	kJ/mol	Joback Method
hvap	84.90	kJ/mol	Joback Method
log10ws	-5.60		Crippen Method
logp	5.447		Crippen Method
mcvol	341.590	ml/mol	McGowan Method
pc	948.50	kPa	Joback Method
rinpola	3207.00		NIST Webbook
rinpola	3207.00		NIST Webbook
tb	877.32	K	Joback Method
tc	1074.12	K	Joback Method
tf	489.25	K	Joback Method
vc	1.327	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1124.56	J/molxK	877.32	Joback Method
cpg	1143.45	J/molxK	910.12	Joback Method
cpg	1161.00	J/molxK	942.92	Joback Method
cpg	1177.23	J/molxK	975.72	Joback Method
cpg	1192.16	J/molxK	1008.52	Joback Method
cpg	1205.79	J/molxK	1041.32	Joback Method
cpg	1218.14	J/molxK	1074.12	Joback Method
dvisc	0.0005231	Paxs	489.25	Joback Method

dvisc	0.0002392	Paxs	553.93	Joback Method
dvisc	0.0001288	Paxs	618.61	Joback Method
dvisc	0.0000780	Paxs	683.28	Joback Method
dvisc	0.0000515	Paxs	747.96	Joback Method
dvisc	0.0000363	Paxs	812.64	Joback Method
dvisc	0.0000270	Paxs	877.32	Joback Method

## Sources

<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=U382279&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382279&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>

## 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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