

# Diglycolic acid, hexyl undecyl ester

<b>Inchi:</b>	InChI=1S/C21H40O5/c1-3-5-7-9-10-11-12-13-15-17-26-21(23)19-24-18-20(22)25-16-14-
<b>InchiKey:</b>	QDMNJJAPJOPMEG-UHFFFAOYSA-N
<b>Formula:</b>	C21H40O5
<b>SMILES:</b>	CCCCCCCCCOC(=O)COCC(=O)OCCCCC
<b>Mol. weight [g/mol]:</b>	372.54

## Physical Properties

Property code	Value	Unit	Source
gf	-446.90	kJ/mol	Joback Method
hf	-1098.59	kJ/mol	Joback Method
hfus	56.91	kJ/mol	Joback Method
hvap	83.06	kJ/mol	Joback Method
log10ws	-5.43		Crippen Method
logp	5.201		Crippen Method
mvol	327.500	ml/mol	McGowan Method
pc	1002.08	kPa	Joback Method
rinpol	3131.00		NIST Webbook
rinpol	3131.00		NIST Webbook
tb	854.88	K	Joback Method
tc	1046.67	K	Joback Method
tf	492.98	K	Joback Method
vc	1.278	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1062.15	J/molxK	854.88	Joback Method
cpg	1142.41	J/molxK	1014.70	Joback Method
cpg	1128.76	J/molxK	982.74	Joback Method
cpg	1113.92	J/molxK	950.77	Joback Method
cpg	1097.88	J/molxK	918.81	Joback Method
cpg	1080.63	J/molxK	886.84	Joback Method
cpg	1154.88	J/molxK	1046.67	Joback Method
dvisc	0.0000343	Paxs	854.88	Joback Method

dvisc	0.0000454	Paxs	794.56	Joback Method
dvisc	0.0000628	Paxs	734.25	Joback Method
dvisc	0.0000922	Paxs	673.93	Joback Method
dvisc	0.0001459	Paxs	613.61	Joback Method
dvisc	0.0002551	Paxs	553.30	Joback Method
dvisc	0.0005115	Paxs	492.98	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=U382063&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382063&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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