

# Diglycolic acid, nonyl undecyl ester

<b>Inchi:</b>	InChI=1S/C24H46O5/c1-3-5-7-9-11-12-14-16-18-20-29-24(26)22-27-21-23(25)28-19-17-
<b>InchiKey:</b>	OEBOMRBYCUYGTE-UHFFFAOYSA-N
<b>Formula:</b>	C24H46O5
<b>SMILES:</b>	CCCCCCCCCOC(=O)COCC(=O)OCCCCCCCCC
<b>Mol. weight [g/mol]:</b>	414.62

## Physical Properties

Property code	Value	Unit	Source
gf	-421.64	kJ/mol	Joback Method
hf	-1160.51	kJ/mol	Joback Method
hfus	64.68	kJ/mol	Joback Method
hvap	89.74	kJ/mol	Joback Method
log10ws	-6.68		Crippen Method
logp	6.371		Crippen Method
mvol	369.770	ml/mol	McGowan Method
pc	841.62	kPa	Joback Method
rinpol	3473.00		NIST Webbook
rinpol	3473.00		NIST Webbook
tb	923.52	K	Joback Method
tc	1134.13	K	Joback Method
tf	526.79	K	Joback Method
vc	1.446	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1249.72	J/molxK	923.52	Joback Method
cpg	1269.63	J/molxK	958.62	Joback Method
cpg	1287.94	J/molxK	993.72	Joback Method
cpg	1304.68	J/molxK	1028.83	Joback Method
cpg	1319.88	J/molxK	1063.93	Joback Method
cpg	1333.55	J/molxK	1099.03	Joback Method
cpg	1345.72	J/molxK	1134.13	Joback Method
dvisc	0.0003557	Paxs	526.79	Joback Method

dvisc	0.0001721	Paxs	592.91	Joback Method
dvisc	0.0000963	Paxs	659.03	Joback Method
dvisc	0.0000599	Paxs	725.15	Joback Method
dvisc	0.0000404	Paxs	791.28	Joback Method
dvisc	0.0000289	Paxs	857.40	Joback Method
dvisc	0.0000217	Paxs	923.52	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=U381866&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381866&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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