

# Diglycolic acid, dodecyl hexyl ester

<b>Inchi:</b>	InChI=1S/C22H42O5/c1-3-5-7-9-10-11-12-13-14-16-18-27-22(24)20-25-19-21(23)26-17-
<b>InchiKey:</b>	WTLKFMMLEYSBMT-UHFFFAOYSA-N
<b>Formula:</b>	C22H42O5
<b>SMILES:</b>	CCCCCCCCCCCCOC(=O)COCC(=O)OCCCCC
<b>Mol. weight [g/mol]:</b>	386.57

## Physical Properties

Property code	Value	Unit	Source
gf	-438.48	kJ/mol	Joback Method
hf	-1119.23	kJ/mol	Joback Method
hfus	59.50	kJ/mol	Joback Method
hvap	85.29	kJ/mol	Joback Method
log10ws	-5.84		Crippen Method
logp	5.591		Crippen Method
mvol	341.590	ml/mol	McGowan Method
pc	943.84	kPa	Joback Method
rinpol	3248.00		NIST Webbook
rinpol	3248.00		NIST Webbook
tb	877.76	K	Joback Method
tc	1074.82	K	Joback Method
tf	504.25	K	Joback Method
vc	1.333	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1124.11	J/molxK	877.76	Joback Method
cpg	1143.04	J/molxK	910.60	Joback Method
cpg	1160.64	J/molxK	943.45	Joback Method
cpg	1176.92	J/molxK	976.29	Joback Method
cpg	1191.91	J/molxK	1009.14	Joback Method
cpg	1205.60	J/molxK	1041.98	Joback Method
cpg	1218.02	J/molxK	1074.82	Joback Method
dvisc	0.0004546	Paxs	504.25	Joback Method

dvisc	0.0002244	Paxs	566.50	Joback Method
dvisc	0.0001273	Paxs	628.75	Joback Method
dvisc	0.0000800	Paxs	691.00	Joback Method
dvisc	0.0000543	Paxs	753.26	Joback Method
dvisc	0.0000391	Paxs	815.51	Joback Method
dvisc	0.0000295	Paxs	877.76	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=U382064&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382064&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

## Legend

<b>cp<sub>g</sub>:</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>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>m<sub>cvol</sub>:</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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