

# Diglycolic acid, hexadecyl 3-methylbutyl ester

<b>Inchi:</b>	InChI=1S/C25H48O5/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-19-29-24(26)21-28-22-25
<b>InchiKey:</b>	OLDKODNEINLUBI-UHFFFAOYSA-N
<b>Formula:</b>	C25H48O5
<b>SMILES:</b>	CCCCCCCCCCCCCCCCOC(=O)COCC(=O)OCCC(C)C
<b>Mol. weight [g/mol]:</b>	428.65

## Physical Properties

Property code	Value	Unit	Source
gf	-415.66	kJ/mol	Joback Method
hf	-1186.43	kJ/mol	Joback Method
hfus	63.74	kJ/mol	Joback Method
hvap	91.58	kJ/mol	Joback Method
log10ws	-6.86		Crippen Method
logp	6.617		Crippen Method
mvol	383.860	ml/mol	McGowan Method
pc	800.24	kPa	Joback Method
rinpol	3548.00		NIST Webbook
rinpol	3548.00		NIST Webbook
tb	945.96	K	Joback Method
tc	1163.54	K	Joback Method
tf	523.06	K	Joback Method
vc	1.496	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1313.62	J/molxK	945.96	Joback Method
cpg	1333.88	J/molxK	982.22	Joback Method
cpg	1352.40	J/molxK	1018.49	Joback Method
cpg	1369.21	J/molxK	1054.75	Joback Method
cpg	1384.32	J/molxK	1091.02	Joback Method
cpg	1397.77	J/molxK	1127.28	Joback Method
cpg	1409.59	J/molxK	1163.54	Joback Method
dvisc	0.0003553	Paxs	523.06	Joback Method

dvisc	0.0001583	Paxs	593.54	Joback Method
dvisc	0.0000837	Paxs	664.03	Joback Method
dvisc	0.0000501	Paxs	734.51	Joback Method
dvisc	0.0000327	Paxs	804.99	Joback Method
dvisc	0.0000229	Paxs	875.48	Joback Method
dvisc	0.0000169	Paxs	945.96	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=U382282&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382282&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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