

# Diglycolic acid, 3,7-dimethyloctyl undecyl ester

Inchi:	InChI=1S/C25H48O5/c1-5-6-7-8-9-10-11-12-13-18-29-24(26)20-28-21-25(27)30-19-17-2
InchiKey:	RIZOIAZAZVIXRA-UHFFFAOYSA-N
Formula:	C25H48O5
SMILES:	CCCCCCCCCOC(=O)COCC(=O)OCCC(C)CCCC(C)C
Mol. weight [g/mol]:	428.65

## Physical Properties

Property code	Value	Unit	Source
gf	-418.10	kJ/mol	Joback Method
hf	-1191.71	kJ/mol	Joback Method
hfus	60.22	kJ/mol	Joback Method
hvap	91.19	kJ/mol	Joback Method
log10ws	-6.62		Crippen Method
logp	6.473		Crippen Method
mvol	383.860	ml/mol	McGowan Method
pc	803.88	kPa	Joback Method
rinpol	3457.00		NIST Webbook
rinpol	3457.00		NIST Webbook
tb	945.52	K	Joback Method
tc	1161.79	K	Joback Method
tf	508.06	K	Joback Method
vc	1.490	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1313.99	J/molxK	945.52	Joback Method
cpg	1334.10	J/molxK	981.57	Joback Method
cpg	1352.48	J/molxK	1017.61	Joback Method
cpg	1369.14	J/molxK	1053.66	Joback Method
cpg	1384.12	J/molxK	1089.70	Joback Method
cpg	1397.45	J/molxK	1125.75	Joback Method
cpg	1409.15	J/molxK	1161.79	Joback Method
dvisc	0.0004093	Paxs	508.06	Joback Method

dvisc	0.0001683	Paxs	580.97	Joback Method
dvisc	0.0000843	Paxs	653.88	Joback Method
dvisc	0.0000486	Paxs	726.79	Joback Method
dvisc	0.0000309	Paxs	799.70	Joback Method
dvisc	0.0000212	Paxs	872.61	Joback Method
dvisc	0.0000154	Paxs	945.52	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=U382152&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382152&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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