

# Diglycolic acid, ethyl heptyl ester

<b>Inchi:</b>	InChI=1S/C13H24O5/c1-3-5-6-7-8-9-18-13(15)11-16-10-12(14)17-4-2/h3-11H2,1-2H3
<b>InchiKey:</b>	YFTXYQVFQWGKBS-UHFFFAOYSA-N
<b>Formula:</b>	C13H24O5
<b>SMILES:</b>	CCCCCCCOC(=O)COCC(=O)OCC
<b>Mol. weight [g/mol]:</b>	260.33

## Physical Properties

Property code	Value	Unit	Source
gf	-514.26	kJ/mol	Joback Method
hf	-933.47	kJ/mol	Joback Method
hfus	36.19	kJ/mol	Joback Method
hvap	65.25	kJ/mol	Joback Method
log10ws	-2.08		Crippen Method
logp	2.080		Crippen Method
mcvol	214.780	ml/mol	McGowan Method
pc	1749.21	kPa	Joback Method
rinpol	2148.00		NIST Webbook
rinpol	2148.00		NIST Webbook
tb	671.84	K	Joback Method
tc	848.38	K	Joback Method
tf	402.82	K	Joback Method
vc	0.830	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.49	J/molxK	671.84	Joback Method
cpg	664.37	J/molxK	818.96	Joback Method
cpg	652.19	J/molxK	789.54	Joback Method
cpg	639.30	J/molxK	760.11	Joback Method
cpg	625.72	J/molxK	730.69	Joback Method
cpg	611.45	J/molxK	701.26	Joback Method
cpg	675.85	J/molxK	848.38	Joback Method
dvisc	0.0001046	Paxs	671.84	Joback Method

dvisc	0.0001350	Paxs	627.00	Joback Method
dvisc	0.0001811	Paxs	582.17	Joback Method
dvisc	0.0002553	Paxs	537.33	Joback Method
dvisc	0.0003829	Paxs	492.49	Joback Method
dvisc	0.0006229	Paxs	447.66	Joback Method
dvisc	0.0011295	Paxs	402.82	Joback Method

## Sources

<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=U381951&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381951&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>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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