

# Diglycolic acid, hexyl octyl ester

<b>Inchi:</b>	InChI=1S/C18H34O5/c1-3-5-7-9-10-12-14-23-18(20)16-21-15-17(19)22-13-11-8-6-4-2/h3
<b>InchiKey:</b>	KNFWOUGCHLBMFI-UHFFFAOYSA-N
<b>Formula:</b>	C18H34O5
<b>SMILES:</b>	CCCCCCCCOC(=O)COCC(=O)OCCCCC
<b>Mol. weight [g/mol]:</b>	330.46

## Physical Properties

Property code	Value	Unit	Source
gf	-472.16	kJ/mol	Joback Method
hf	-1036.67	kJ/mol	Joback Method
hfus	49.14	kJ/mol	Joback Method
hvap	76.38	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	4.030		Crippen Method
mvol	285.230	ml/mol	McGowan Method
pc	1213.20	kPa	Joback Method
rinpol	2754.00		NIST Webbook
rinpol	2754.00		NIST Webbook
tb	786.24	K	Joback Method
tc	967.32	K	Joback Method
tf	459.17	K	Joback Method
vc	1.109	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	880.48	J/molxK	786.24	Joback Method
cpg	956.81	J/molxK	937.14	Joback Method
cpg	943.48	J/molxK	906.96	Joback Method
cpg	929.18	J/molxK	876.78	Joback Method
cpg	913.92	J/molxK	846.60	Joback Method
cpg	897.68	J/molxK	816.42	Joback Method
cpg	969.19	J/molxK	967.32	Joback Method
dvisc	0.0000532	Paxs	786.24	Joback Method

dvisc	0.0000698	Paxs	731.73	Joback Method
dvisc	0.0000957	Paxs	677.22	Joback Method
dvisc	0.0001386	Paxs	622.71	Joback Method
dvisc	0.0002154	Paxs	568.19	Joback Method
dvisc	0.0003677	Paxs	513.68	Joback Method
dvisc	0.0007129	Paxs	459.17	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U382114&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382114&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>
<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>

## 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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