

# Diglycolic acid, heptyl oct-4-yl ester

<b>Inchi:</b>	InChI=1S/C19H36O5/c1-4-7-9-10-11-14-23-18(20)15-22-16-19(21)24-17(12-6-3)13-8-5-2
<b>InchiKey:</b>	WWICSGWZEUEHIH-UHFFFAOYSA-N
<b>Formula:</b>	C19H36O5
<b>SMILES:</b>	CCCCCCCOC(=O)COCC(=O)OC(CCC)CCCC
<b>Mol. weight [g/mol]:</b>	344.49

## Physical Properties

Property code	Value	Unit	Source
gf	-466.18	kJ/mol	Joback Method
hf	-1062.59	kJ/mol	Joback Method
hfus	48.20	kJ/mol	Joback Method
hvap	78.22	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	4.419		Crippen Method
mvol	299.320	ml/mol	McGowan Method
pc	1142.12	kPa	Joback Method
rinpol	2701.00		NIST Webbook
rinpol	2701.00		NIST Webbook
tb	808.68	K	Joback Method
tc	993.30	K	Joback Method
tf	455.44	K	Joback Method
vc	1.159	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	940.75	J/molxK	808.68	Joback Method
cpg	958.44	J/molxK	839.45	Joback Method
cpg	975.07	J/molxK	870.22	Joback Method
cpg	990.65	J/molxK	900.99	Joback Method
cpg	1005.16	J/molxK	931.76	Joback Method
cpg	1018.64	J/molxK	962.53	Joback Method
cpg	1031.06	J/molxK	993.30	Joback Method
dvisc	0.0007490	Paxs	455.44	Joback Method

dvisc	0.0003527	Paxs	514.31	Joback Method
dvisc	0.0001939	Paxs	573.19	Joback Method
dvisc	0.0001192	Paxs	632.06	Joback Method
dvisc	0.0000796	Paxs	690.93	Joback Method
dvisc	0.0000566	Paxs	749.81	Joback Method
dvisc	0.0000423	Paxs	808.68	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=U382024&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382024&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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