

# Diglycolic acid, heptyl nonyl ester

<b>Inchi:</b>	InChI=1S/C20H38O5/c1-3-5-7-9-10-12-14-16-25-20(22)18-23-17-19(21)24-15-13-11-8-6
<b>InchiKey:</b>	ANGCIFVLAQAUMW-UHFFFAOYSA-N
<b>Formula:</b>	C20H38O5
<b>SMILES:</b>	CCCCCCCCCOC(=O)COCC(=O)OCCCCCCC
<b>Mol. weight [g/mol]:</b>	358.51

## Physical Properties

Property code	Value	Unit	Source
gf	-455.32	kJ/mol	Joback Method
hf	-1077.95	kJ/mol	Joback Method
hfus	54.32	kJ/mol	Joback Method
hvap	80.84	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	4.810		Crippen Method
mvol	313.410	ml/mol	McGowan Method
pc	1065.87	kPa	Joback Method
rinpol	3004.00		NIST Webbook
rinpol	3004.00		NIST Webbook
tb	832.00	K	Joback Method
tc	1019.41	K	Joback Method
tf	481.71	K	Joback Method
vc	1.222	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1000.84	J/molxK	832.00	Joback Method
cpg	1018.88	J/molxK	863.24	Joback Method
cpg	1035.80	J/molxK	894.47	Joback Method
cpg	1051.59	J/molxK	925.71	Joback Method
cpg	1066.26	J/molxK	956.94	Joback Method
cpg	1079.84	J/molxK	988.18	Joback Method
cpg	1092.31	J/molxK	1019.41	Joback Method
dvisc	0.0005736	Paxs	481.71	Joback Method

dvisc	0.0002891	Paxs	540.09	Joback Method
dvisc	0.0001666	Paxs	598.47	Joback Method
dvisc	0.0001059	Paxs	656.86	Joback Method
dvisc	0.0000725	Paxs	715.24	Joback Method
dvisc	0.0000525	Paxs	773.62	Joback Method
dvisc	0.0000398	Paxs	832.00	Joback Method

## Sources

<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=U381957&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381957&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>

## Legend

<b>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>w<sub>s</sub>:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mc<sub>vol</sub>:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rin<sub>pol</sub>:</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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