

# Diglycolic acid, decyl neopentyl ester

**Inchi:** InChI=1S/C19H36O5/c1-5-6-7-8-9-10-11-12-13-23-17(20)14-22-15-18(21)24-16-19(2,3)4  
**InchiKey:** IIWJIVFHXQNTOU-UHFFFAOYSA-N  
**Formula:** C19H36O5  
**SMILES:** CCCCCCCCCCOC(=O)COCC(=O)OCC(C)(C)C  
**Mol. weight [g/mol]:** 344.49

## Physical Properties

Property code	Value	Unit	Source
gf	-460.90	kJ/mol	Joback Method
hf	-1066.06	kJ/mol	Joback Method
hfus	44.31	kJ/mol	Joback Method
hvap	77.31	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	4.276		Crippen Method
mvol	299.320	ml/mol	McGowan Method
pc	1150.65	kPa	Joback Method
rinpol	2747.00		NIST Webbook
rinpol	2747.00		NIST Webbook
tb	805.89	K	Joback Method
tc	991.96	K	Joback Method
tf	472.86	K	Joback Method
vc	1.155	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	941.33	J/molxK	805.89	Joback Method
cpg	958.94	J/molxK	836.90	Joback Method
cpg	975.48	J/molxK	867.91	Joback Method
cpg	990.99	J/molxK	898.92	Joback Method
cpg	1005.48	J/molxK	929.94	Joback Method
cpg	1018.97	J/molxK	960.95	Joback Method
cpg	1031.48	J/molxK	991.96	Joback Method
dvisc	0.0006049	Paxs	472.86	Joback Method

dvisc	0.0002972	Paxs	528.37	Joback Method
dvisc	0.0001672	Paxs	583.87	Joback Method
dvisc	0.0001039	Paxs	639.38	Joback Method
dvisc	0.0000697	Paxs	694.88	Joback Method
dvisc	0.0000496	Paxs	750.38	Joback Method
dvisc	0.0000370	Paxs	805.89	Joback Method

## Sources

<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=U381922&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381922&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>

## 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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