

# Diglycolic acid, di(oct-4-yl) ester

<b>Inchi:</b>	InChI=1S/C20H38O5/c1-5-9-13-17(11-7-3)24-19(21)15-23-16-20(22)25-18(12-8-4)14-10
<b>InchiKey:</b>	AKHQLZSSKIHFMM-UHFFFAOYSA-N
<b>Formula:</b>	C20H38O5
<b>SMILES:</b>	CCCCC(CCC)OC(=O)COCC(=O)OC(CCC)CCCC
<b>Mol. weight [g/mol]:</b>	358.51

## Physical Properties

Property code	Value	Unit	Source
gf	-460.20	kJ/mol	Joback Method
hf	-1088.51	kJ/mol	Joback Method
hfus	47.27	kJ/mol	Joback Method
hvap	80.06	kJ/mol	Joback Method
log10ws	-5.23		Crippen Method
logp	4.807		Crippen Method
mvol	313.410	ml/mol	McGowan Method
pc	1077.10	kPa	Joback Method
rinpol	2642.00		NIST Webbook
rinpol	2642.00		NIST Webbook
tb	831.12	K	Joback Method
tc	1019.53	K	Joback Method
tf	451.71	K	Joback Method
vc	1.210	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1001.80	J/molxK	831.12	Joback Method
cpg	1019.93	J/molxK	862.52	Joback Method
cpg	1036.90	J/molxK	893.92	Joback Method
cpg	1052.72	J/molxK	925.33	Joback Method
cpg	1067.40	J/molxK	956.73	Joback Method
cpg	1080.94	J/molxK	988.13	Joback Method
cpg	1093.35	J/molxK	1019.53	Joback Method
dvisc	0.0007901	Paxs	451.71	Joback Method

dvisc	0.0003376	Paxs	514.95	Joback Method
dvisc	0.0001737	Paxs	578.18	Joback Method
dvisc	0.0001019	Paxs	641.41	Joback Method
dvisc	0.0000658	Paxs	704.65	Joback Method
dvisc	0.0000456	Paxs	767.88	Joback Method
dvisc	0.0000335	Paxs	831.12	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=U382034&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382034&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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