

# Diglycolic acid, 4-methoxybenzyl octyl ester

<b>Inchi:</b>	InChI=1S/C20H30O6/c1-3-4-5-6-7-8-13-25-19(21)15-24-16-20(22)26-14-17-9-11-18(23-24)
<b>InchiKey:</b>	HANKYJXHIVGYMA-UHFFFAOYSA-N
<b>Formula:</b>	C20H30O6
<b>SMILES:</b>	CCCCCCCCOC(=O)COCC(=O)OCc1ccc(OC)cc1
<b>Mol. weight [g/mol]:</b>	366.45

## Physical Properties

Property code	Value	Unit	Source
gf	-457.54	kJ/mol	Joback Method
hf	-985.11	kJ/mol	Joback Method
hfus	49.16	kJ/mol	Joback Method
hvap	86.18	kJ/mol	Joback Method
log10ws	-4.31		Crippen Method
logp	3.659		Crippen Method
mvol	295.520	ml/mol	McGowan Method
pc	1308.95	kPa	Joback Method
rinpol	3421.00		NIST Webbook
rinpol	3421.00		NIST Webbook
tb	886.08	K	Joback Method
tc	1089.73	K	Joback Method
tf	542.88	K	Joback Method
vc	1.131	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	936.21	J/molxK	886.08	Joback Method
cpg	998.40	J/molxK	1055.79	Joback Method
cpg	988.62	J/molxK	1021.84	Joback Method
cpg	977.51	J/molxK	987.90	Joback Method
cpg	965.06	J/molxK	953.96	Joback Method
cpg	951.30	J/molxK	920.02	Joback Method
cpg	1006.86	J/molxK	1089.73	Joback Method
dvisc	0.0000307	Paxs	886.08	Joback Method

dvisc	0.0000392	Paxs	828.88	Joback Method
dvisc	0.0000520	Paxs	771.68	Joback Method
dvisc	0.0000722	Paxs	714.48	Joback Method
dvisc	0.0001060	Paxs	657.28	Joback Method
dvisc	0.0001676	Paxs	600.08	Joback Method
dvisc	0.0002917	Paxs	542.88	Joback Method

## Sources

<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=U382253&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382253&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

<b>cp<sub>g</sub>:</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>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>m<sub>cvol</sub>:</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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