

# Diglycolic acid, octyl 2,4,4-trimethylpentyl ester

Inchi:	InChI=1S/C20H38O5/c1-6-7-8-9-10-11-12-24-18(21)15-23-16-19(22)25-14-17(2)13-20(3)
InchiKey:	OUZUENMJYWROCL-UHFFFAOYSA-N
Formula:	C20H38O5
SMILES:	CCCCCCCCOC(=O)COCC(=O)OCC(C)CC(C)(C)C
Mol. weight [g/mol]:	358.51

## Physical Properties

Property code	Value	Unit	Source
gf	-454.92	kJ/mol	Joback Method
hf	-1091.98	kJ/mol	Joback Method
hfus	43.38	kJ/mol	Joback Method
hvap	79.15	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	4.522		Crippen Method
mcvol	313.410	ml/mol	McGowan Method
pc	1084.92	kPa	Joback Method
rinpol	2811.00		NIST Webbook
rinpol	2811.00		NIST Webbook
tb	828.33	K	Joback Method
tc	1017.82	K	Joback Method
tf	469.13	K	Joback Method
vc	1.204	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1002.14	J/molxK	828.33	Joback Method
cpg	1020.16	J/molxK	859.91	Joback Method
cpg	1037.05	J/molxK	891.49	Joback Method
cpg	1052.82	J/molxK	923.08	Joback Method
cpg	1067.49	J/molxK	954.66	Joback Method
cpg	1081.09	J/molxK	986.24	Joback Method
cpg	1093.65	J/molxK	1017.82	Joback Method
dvisc	0.0006309	Paxs	469.13	Joback Method

dvisc	0.0002825	Paxs	529.00	Joback Method
dvisc	0.0001489	Paxs	588.86	Joback Method
dvisc	0.0000884	Paxs	648.73	Joback Method
dvisc	0.0000573	Paxs	708.60	Joback Method
dvisc	0.0000397	Paxs	768.46	Joback Method
dvisc	0.0000290	Paxs	828.33	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U382043&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382043&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>mccvol:</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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