

# Diglycolic acid, 3-methylphenyl octyl ester

<b>Inchi:</b>	InChI=1S/C19H28O5/c1-3-4-5-6-7-8-12-23-18(20)14-22-15-19(21)24-17-11-9-10-16(2)13
<b>InchiKey:</b>	MTJXELKXUDRZCU-UHFFFAOYSA-N
<b>Formula:</b>	C19H28O5
<b>SMILES:</b>	CCCCCCCCOC(=O)COCC(=O)Oc1cccc(C)c1
<b>Mol. weight [g/mol]:</b>	336.42

## Physical Properties

Property code	Value	Unit	Source
gf	-360.96	kJ/mol	Joback Method
hf	-832.25	kJ/mol	Joback Method
hfus	45.38	kJ/mol	Joback Method
hvap	81.55	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	3.821		Crippen Method
mcvol	275.560	ml/mol	McGowan Method
pc	1422.92	kPa	Joback Method
rinpol	3015.00		NIST Webbook
rinpol	3015.00		NIST Webbook
tb	840.78	K	Joback Method
tc	1041.20	K	Joback Method
tf	509.38	K	Joback Method
vc	1.058	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	848.17	J/molxK	840.78	Joback Method
cpg	863.62	J/molxK	874.18	Joback Method
cpg	877.92	J/molxK	907.59	Joback Method
cpg	891.07	J/molxK	940.99	Joback Method
cpg	903.09	J/molxK	974.39	Joback Method
cpg	913.97	J/molxK	1007.79	Joback Method
cpg	923.73	J/molxK	1041.20	Joback Method
dvisc	0.0004609	Paxs	509.38	Joback Method

dvisc	0.0002620	Paxs	564.61	Joback Method
dvisc	0.0001648	Paxs	619.85	Joback Method
dvisc	0.0001118	Paxs	675.08	Joback Method
dvisc	0.0000804	Paxs	730.31	Joback Method
dvisc	0.0000606	Paxs	785.55	Joback Method
dvisc	0.0000474	Paxs	840.78	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=U382105&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382105&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>

## 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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