

# Diglycolic acid, hexyl 3-methylphenyl ester

<b>Inchi:</b>	InChI=1S/C17H24O5/c1-3-4-5-6-10-21-16(18)12-20-13-17(19)22-15-9-7-8-14(2)11-15/h
<b>InchiKey:</b>	DIFSUVCSJUWIEZ-UHFFFAOYSA-N
<b>Formula:</b>	C17H24O5
<b>SMILES:</b>	CCCCCOC(=O)COCC(=O)Oc1cccc(C)c1
<b>Mol. weight [g/mol]:</b>	308.37

## Physical Properties

Property code	Value	Unit	Source
gf	-377.80	kJ/mol	Joback Method
hf	-790.97	kJ/mol	Joback Method
hfus	40.20	kJ/mol	Joback Method
hvap	77.10	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.041		Crippen Method
mvol	247.380	ml/mol	McGowan Method
pc	1653.80	kPa	Joback Method
rinpol	2760.00		NIST Webbook
rinpol	2760.00		NIST Webbook
tb	795.02	K	Joback Method
tc	995.27	K	Joback Method
tf	486.84	K	Joback Method
vc	0.946	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	732.69	J/molxK	795.02	Joback Method
cpg	797.27	J/molxK	961.90	Joback Method
cpg	786.44	J/molxK	928.52	Joback Method
cpg	774.58	J/molxK	895.15	Joback Method
cpg	761.66	J/molxK	861.77	Joback Method
cpg	747.70	J/molxK	828.40	Joback Method
cpg	807.05	J/molxK	995.27	Joback Method
dvisc	0.0000624	Paxs	795.02	Joback Method

dvisc	0.0000792	Paxs	743.66	Joback Method
dvisc	0.0001043	Paxs	692.29	Joback Method
dvisc	0.0001434	Paxs	640.93	Joback Method
dvisc	0.0002084	Paxs	589.57	Joback Method
dvisc	0.0003254	Paxs	538.20	Joback Method
dvisc	0.0005581	Paxs	486.84	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=U382103&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382103&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

## Legend

<b>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>w<sub>s</sub>:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</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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