

# Diglycolic acid, 2,5-dimethylphenyl hexyl ester

<b>Inchi:</b>	InChI=1S/C18H26O5/c1-4-5-6-7-10-22-17(19)12-21-13-18(20)23-16-11-14(2)8-9-15(16)3
<b>InchiKey:</b>	HZTFCUMIWAZXOY-UHFFFAOYSA-N
<b>Formula:</b>	C18H26O5
<b>SMILES:</b>	CCCCCOC(=O)COCC(=O)Oc1cc(C)ccc1C
<b>Mol. weight [g/mol]:</b>	322.40

## Physical Properties

Property code	Value	Unit	Source
gf	-379.01	kJ/mol	Joback Method
hf	-823.08	kJ/mol	Joback Method
hfus	42.40	kJ/mol	Joback Method
hvap	79.98	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	3.349		Crippen Method
mvol	261.470	ml/mol	McGowan Method
pc	1514.03	kPa	Joback Method
rinpol	2828.00		NIST Webbook
rinpol	2828.00		NIST Webbook
tb	822.88	K	Joback Method
tc	1023.72	K	Joback Method
tf	510.63	K	Joback Method
vc	1.002	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	789.23	J/molxK	822.88	Joback Method
cpg	804.38	J/molxK	856.35	Joback Method
cpg	818.44	J/molxK	889.83	Joback Method
cpg	831.39	J/molxK	923.30	Joback Method
cpg	843.23	J/molxK	956.78	Joback Method
cpg	853.98	J/molxK	990.25	Joback Method
cpg	863.61	J/molxK	1023.72	Joback Method
dvisc	0.0004391	Paxs	510.63	Joback Method

dvisc	0.0002647	Paxs	562.67	Joback Method
dvisc	0.0001738	Paxs	614.71	Joback Method
dvisc	0.0001219	Paxs	666.75	Joback Method
dvisc	0.0000900	Paxs	718.80	Joback Method
dvisc	0.0000692	Paxs	770.84	Joback Method
dvisc	0.0000550	Paxs	822.88	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=U382708&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382708&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

Latest version available from:

<https://www.chemeo.com/cid/81-958-9/Diglycolic-acid-2-5-dimethylphenyl-hexyl-ester.pdf>

Generated by Cheméo on 2024-04-18 14:38:06.492085038 +0000 UTC m=+15740335.412662361.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.