

# Diglycolic acid, 4-chlorophenyl octyl ester

<b>Inchi:</b>	InChI=1S/C18H25ClO5/c1-2-3-4-5-6-7-12-23-17(20)13-22-14-18(21)24-16-10-8-15(19)9
<b>InchiKey:</b>	BASDQKQWOIHHSX-UHFFFAOYSA-N
<b>Formula:</b>	C18H25ClO5
<b>SMILES:</b>	CCCCCCCCOC(=O)COCC(=O)Oc1ccc(Cl)cc1
<b>Mol. weight [g/mol]:</b>	356.84

## Physical Properties

Property code	Value	Unit	Source
gf	-381.31	kJ/mol	Joback Method
hf	-827.35	kJ/mol	Joback Method
hfus	46.99	kJ/mol	Joback Method
hvap	83.71	kJ/mol	Joback Method
log10ws	-4.61		Crippen Method
logp	4.166		Crippen Method
mvol	273.710	ml/mol	McGowan Method
pc	1488.44	kPa	Joback Method
rinpol	3133.00		NIST Webbook
rinpol	3133.00		NIST Webbook
tb	855.33	K	Joback Method
tc	1060.14	K	Joback Method
tf	528.03	K	Joback Method
vc	1.050	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	816.44	J/molxK	855.33	Joback Method
cpg	830.50	J/molxK	889.47	Joback Method
cpg	843.41	J/molxK	923.60	Joback Method
cpg	855.18	J/molxK	957.74	Joback Method
cpg	865.84	J/molxK	991.87	Joback Method
cpg	875.37	J/molxK	1026.01	Joback Method
cpg	883.79	J/molxK	1060.14	Joback Method
dvisc	0.0004196	Paxs	528.03	Joback Method

dvisc	0.0002457	Paxs	582.58	Joback Method
dvisc	0.0001577	Paxs	637.13	Joback Method
dvisc	0.0001086	Paxs	691.68	Joback Method
dvisc	0.0000789	Paxs	746.23	Joback Method
dvisc	0.0000599	Paxs	800.78	Joback Method
dvisc	0.0000471	Paxs	855.33	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U381783&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381783&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>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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