

# Diglycolic acid, 2,6-dichlorophenyl octyl ester

<b>Inchi:</b>	InChI=1S/C18H24Cl2O5/c1-2-3-4-5-6-7-11-24-16(21)12-23-13-17(22)25-18-14(19)9-8-10
<b>InchiKey:</b>	KMJSYMWRSVLRDU-UHFFFAOYSA-N
<b>Formula:</b>	C18H24Cl2O5
<b>SMILES:</b>	CCCCCCCCOC(=O)COCC(=O)Oc1c(Cl)cccc1Cl
<b>Mol. weight [g/mol]:</b>	391.29

## Physical Properties

Property code	Value	Unit	Source
gf	-402.87	kJ/mol	Joback Method
hf	-854.56	kJ/mol	Joback Method
hfus	50.79	kJ/mol	Joback Method
hvap	88.75	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	4.819		Crippen Method
mvol	285.950	ml/mol	McGowan Method
pc	1430.46	kPa	Joback Method
rinpol	3245.00		NIST Webbook
rinpol	3245.00		NIST Webbook
tb	897.74	K	Joback Method
tc	1108.53	K	Joback Method
tf	570.47	K	Joback Method
vc	1.099	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	839.69	J/molxK	897.74	Joback Method
cpg	852.42	J/molxK	932.87	Joback Method
cpg	863.96	J/molxK	968.00	Joback Method
cpg	874.31	J/molxK	1003.13	Joback Method
cpg	883.48	J/molxK	1038.26	Joback Method
cpg	891.46	J/molxK	1073.39	Joback Method
cpg	898.27	J/molxK	1108.53	Joback Method
dvisc	0.0003039	Paxs	570.47	Joback Method

dvisc	0.0001881	Paxs	625.01	Joback Method
dvisc	0.0001257	Paxs	679.56	Joback Method
dvisc	0.0000892	Paxs	734.11	Joback Method
dvisc	0.0000664	Paxs	788.65	Joback Method
dvisc	0.0000513	Paxs	843.19	Joback Method
dvisc	0.0000409	Paxs	897.74	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=U382303&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382303&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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