

# Diglycolic acid, 2,6-dichlorophenyl heptyl ester

Inchi:	InChI=1S/C17H22Cl2O5/c1-2-3-4-5-6-10-23-15(20)11-22-12-16(21)24-17-13(18)8-7-9-14
InchiKey:	SMEKULMSLOURME-UHFFFAOYSA-N
Formula:	C17H22Cl2O5
SMILES:	CCCCCCCOC(=O)COCC(=O)Oc1c(Cl)cccc1Cl
Mol. weight [g/mol]:	377.26

## Physical Properties

Property code	Value	Unit	Source
gf	-411.29	kJ/mol	Joback Method
hf	-833.92	kJ/mol	Joback Method
hfus	48.20	kJ/mol	Joback Method
hvap	86.53	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.429		Crippen Method
mvol	271.860	ml/mol	McGowan Method
pc	1540.29	kPa	Joback Method
rinpol	3124.00		NIST Webbook
rinpol	3124.00		NIST Webbook
tb	874.86	K	Joback Method
tc	1084.98	K	Joback Method
tf	559.20	K	Joback Method
vc	1.044	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	782.22	J/molxK	874.86	Joback Method
cpg	794.77	J/molxK	909.88	Joback Method
cpg	806.18	J/molxK	944.90	Joback Method
cpg	816.46	J/molxK	979.92	Joback Method
cpg	825.61	J/molxK	1014.94	Joback Method
cpg	833.63	J/molxK	1049.96	Joback Method
cpg	840.51	J/molxK	1084.98	Joback Method
dvisc	0.0003376	Paxs	559.20	Joback Method

dvisc	0.0002114	Paxs	611.81	Joback Method
dvisc	0.0001426	Paxs	664.42	Joback Method
dvisc	0.0001019	Paxs	717.03	Joback Method
dvisc	0.0000762	Paxs	769.64	Joback Method
dvisc	0.0000592	Paxs	822.25	Joback Method
dvisc	0.0000474	Paxs	874.86	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=U382302&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382302&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>

## 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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