

# Terephthalic acid, 2-chloropropyl hexyl ester

<b>Inchi:</b>	InChI=1S/C17H23ClO4/c1-3-4-5-6-11-21-16(19)14-7-9-15(10-8-14)17(20)22-12-13(2)18
<b>InchiKey:</b>	JRNSUEZMONBKGI-UHFFFAOYSA-N
<b>Formula:</b>	C17H23ClO4
<b>SMILES:</b>	CCCCCOC(=O)c1ccc(C(=O)OCC(C)Cl)cc1
<b>Mol. weight [g/mol]:</b>	326.81

## Physical Properties

Property code	Value	Unit	Source
gf	-287.17	kJ/mol	Joback Method
hf	-679.77	kJ/mol	Joback Method
hfus	39.69	kJ/mol	Joback Method
hvap	78.68	kJ/mol	Joback Method
log10ws	-5.15		Crippen Method
logp	4.208		Crippen Method
mcvol	253.750	ml/mol	McGowan Method
pc	1637.78	kPa	Joback Method
rinqol	2371.00		NIST Webbook
tb	809.59	K	Joback Method
tc	1016.62	K	Joback Method
tf	479.53	K	Joback Method
vc	0.971	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	731.89	J/molxK	809.59	Joback Method
cpg	746.34	J/molxK	844.09	Joback Method
cpg	759.73	J/molxK	878.60	Joback Method
cpg	772.07	J/molxK	913.10	Joback Method
cpg	783.39	J/molxK	947.61	Joback Method
cpg	793.70	J/molxK	982.11	Joback Method
cpg	803.02	J/molxK	1016.62	Joback Method
dvisc	0.0007413	Paxs	479.53	Joback Method
dvisc	0.0004031	Paxs	534.54	Joback Method

dvisc	0.0002455	Paxs	589.55	Joback Method
dvisc	0.0001628	Paxs	644.56	Joback Method
dvisc	0.0001151	Paxs	699.57	Joback Method
dvisc	0.0000857	Paxs	754.58	Joback Method
dvisc	0.0000663	Paxs	809.59	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=U356172&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356172&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>

## 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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