

# Terephthalic acid, 2,2-dichloroethyl undecyl ester

Inchi:	InChI=1S/C21H30Cl2O4/c1-2-3-4-5-6-7-8-9-10-15-26-20(24)17-11-13-18(14-12-17)21(2)
InchiKey:	NVKZMLDDQDJMCF-UHFFFAOYSA-N
Formula:	C21H30Cl2O4
SMILES:	CCCCCCCCCOC(=O)c1ccc(C(=O)OCC(Cl)Cl)cc1
Mol. weight [g/mol]:	417.37

## Physical Properties

Property code	Value	Unit	Source
gf	-265.42	kJ/mol	Joback Method
hf	-778.07	kJ/mol	Joback Method
hfus	54.24	kJ/mol	Joback Method
hvap	91.97	kJ/mol	Joback Method
log10ws	-7.47		Crippen Method
logp	6.335		Crippen Method
mvol	322.350	ml/mol	McGowan Method
pc	1195.65	kPa	Joback Method
rinpol	2947.00		NIST Webbook
rinpol	2947.00		NIST Webbook
tb	938.54	K	Joback Method
tc	1152.87	K	Joback Method
tf	554.53	K	Joback Method
vc	1.244	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	989.93	J/molxK	938.54	Joback Method
cpg	1047.93	J/molxK	1117.15	Joback Method
cpg	1038.69	J/molxK	1081.42	Joback Method
cpg	1028.30	J/molxK	1045.70	Joback Method
cpg	1016.74	J/molxK	1009.98	Joback Method
cpg	1003.96	J/molxK	974.26	Joback Method
cpg	1056.06	J/molxK	1152.87	Joback Method
dvisc	0.0000315	Paxs	938.54	Joback Method

dvisc	0.0000411	Paxs	874.54	Joback Method
dvisc	0.0000558	Paxs	810.54	Joback Method
dvisc	0.0000798	Paxs	746.53	Joback Method
dvisc	0.0001221	Paxs	682.53	Joback Method
dvisc	0.0002040	Paxs	618.53	Joback Method
dvisc	0.0003839	Paxs	554.53	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=U356250&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356250&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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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