

# Phthalic acid, 2,4,5-trichlorophenyl undecyl ester

Inchi:	InChI=1S/C25H29Cl3O4/c1-2-3-4-5-6-7-8-9-12-15-31-24(29)18-13-10-11-14-19(18)25(30)
InchiKey:	FRYUVXZNXHRGHE-UHFFFAOYSA-N
Formula:	C25H29Cl3O4
SMILES:	CCCCCCCCCOC(=O)c1ccccc1C(=O)Oc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]:	499.85

## Physical Properties

Property code	Value	Unit	Source
gf	-157.71	kJ/mol	Joback Method
hf	-668.97	kJ/mol	Joback Method
hfus	65.20	kJ/mol	Joback Method
hvap	109.91	kJ/mol	Joback Method
log10ws	-10.04		Crippen Method
logp	8.554		Crippen Method
mvol	367.190	ml/mol	McGowan Method
pc	1085.63	kPa	Joback Method
rinpol	3433.00		NIST Webbook
rinpol	3433.00		NIST Webbook
tb	1109.55	K	Joback Method
tc	1358.42	K	Joback Method
tf	708.51	K	Joback Method
vc	1.415	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1133.94	J/molxK	1109.55	Joback Method
cpg	1168.26	J/molxK	1316.94	Joback Method
cpg	1164.32	J/molxK	1275.46	Joback Method
cpg	1158.97	J/molxK	1233.98	Joback Method
cpg	1152.17	J/molxK	1192.51	Joback Method
cpg	1143.84	J/molxK	1151.03	Joback Method
cpg	1170.85	J/molxK	1358.42	Joback Method
dvisc	0.0000176	Paxs	1109.55	Joback Method

dvisc	0.0000219	Paxs	1042.71	Joback Method
dvisc	0.0000281	Paxs	975.87	Joback Method
dvisc	0.0000373	Paxs	909.03	Joback Method
dvisc	0.0000519	Paxs	842.19	Joback Method
dvisc	0.0000764	Paxs	775.35	Joback Method
dvisc	0.0001210	Paxs	708.51	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=U357051&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U357051&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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