

# Phthalic acid, 2-chloropropyl pentadecyl ester

**Inchi:** InChI=1S/C26H41ClO4/c1-3-4-5-6-7-8-9-10-11-12-13-14-17-20-30-25(28)23-18-15-16-19  
**InchiKey:** AUYOIZNOHPOJHZ-UHFFFAOYSA-N  
**Formula:** C26H41ClO4  
**SMILES:** CCCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCC(C)Cl  
**Mol. weight [g/mol]:** 453.05

## Physical Properties

Property code	Value	Unit	Source
gf	-211.39	kJ/mol	Joback Method
hf	-865.53	kJ/mol	Joback Method
hfus	63.00	kJ/mol	Joback Method
hvap	98.72	kJ/mol	Joback Method
log10ws	-8.92		Crippen Method
logp	7.719		Crippen Method
mvol	380.560	ml/mol	McGowan Method
pc	899.10	kPa	Joback Method
rinpol	3167.00		NIST Webbook
rinpol	3167.00		NIST Webbook
tb	1015.51	K	Joback Method
tc	1244.39	K	Joback Method
tf	580.96	K	Joback Method
vc	1.474	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1270.07	J/molxK	1015.51	Joback Method
cpg	1336.12	J/molxK	1206.24	Joback Method
cpg	1325.88	J/molxK	1168.10	Joback Method
cpg	1314.22	J/molxK	1129.95	Joback Method
cpg	1301.07	J/molxK	1091.80	Joback Method
cpg	1286.37	J/molxK	1053.66	Joback Method
cpg	1345.00	J/molxK	1244.39	Joback Method
dvisc	0.0000174	Paxs	1015.51	Joback Method

dvisc	0.0000229	Paxs	943.08	Joback Method
dvisc	0.0000317	Paxs	870.66	Joback Method
dvisc	0.0000466	Paxs	798.23	Joback Method
dvisc	0.0000739	Paxs	725.81	Joback Method
dvisc	0.0001298	Paxs	653.38	Joback Method
dvisc	0.0002622	Paxs	580.96	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=U356836&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356836&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>cp<sub>g</sub>:</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>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</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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