

# Phthalic acid, 2-propylphenyl tridecyl ester

<b>Inchi:</b>	InChI=1S/C30H42O4/c1-3-5-6-7-8-9-10-11-12-13-18-24-33-29(31)26-21-15-16-22-27(26)
<b>InchiKey:</b>	ZGRPZNDMANNUIT-UHFFFAOYSA-N
<b>Formula:</b>	C30H42O4
<b>SMILES:</b>	CCCCCCCCCCCCOC(=O)c1ccccc1C(=O)Oc1ccccc1CCC
<b>Mol. weight [g/mol]:</b>	466.65

## Physical Properties

Property code	Value	Unit	Source
gf	-60.56	kJ/mol	Joback Method
hf	-702.01	kJ/mol	Joback Method
hfus	66.33	kJ/mol	Joback Method
hvap	106.56	kJ/mol	Joback Method
log10ws	-10.05		Crippen Method
logp	8.326		Crippen Method
mvol	400.920	ml/mol	McGowan Method
pc	878.44	kPa	Joback Method
rinpol	3338.00		NIST Webbook
rinpol	3338.00		NIST Webbook
tb	1101.70	K	Joback Method
tc	1351.81	K	Joback Method
tf	650.06	K	Joback Method
vc	1.548	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1383.47	J/molxK	1101.70	Joback Method
cpg	1398.34	J/molxK	1143.38	Joback Method
cpg	1411.38	J/molxK	1185.07	Joback Method
cpg	1422.69	J/molxK	1226.75	Joback Method
cpg	1432.37	J/molxK	1268.44	Joback Method
cpg	1440.51	J/molxK	1310.12	Joback Method
cpg	1447.21	J/molxK	1351.81	Joback Method
dvisc	0.0001479	Paxs	650.06	Joback Method

dvisc	0.0000801	Paxs	725.33	Joback Method
dvisc	0.0000487	Paxs	800.61	Joback Method
dvisc	0.0000323	Paxs	875.88	Joback Method
dvisc	0.0000228	Paxs	951.15	Joback Method
dvisc	0.0000170	Paxs	1026.43	Joback Method
dvisc	0.0000132	Paxs	1101.70	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=U357028&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U357028&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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