

# Phthalic acid, tetradecyl 2,4,4-trimethylpentyl ester

Inchi:	InChI=1S/C30H50O4/c1-6-7-8-9-10-11-12-13-14-15-16-19-22-33-28(31)26-20-17-18-21-
InchiKey:	ZBDCGJHQAMMZQX-UHFFFAOYSA-N
Formula:	C30H50O4
SMILES:	CCCCCCCCCCCCCOC(=O)c1cccc1C(=O)OCC(C)CC(C)(C)C
Mol. weight [g/mol]:	474.72

## Physical Properties

Property code	Value	Unit	Source
gf	-162.94	kJ/mol	Joback Method
hf	-941.10	kJ/mol	Joback Method
hfus	61.74	kJ/mol	Joback Method
hvap	101.94	kJ/mol	Joback Method
log10ws	-9.85		Crippen Method
logp	8.774		Crippen Method
mvol	424.680	ml/mol	McGowan Method
pc	745.29	kPa	Joback Method
rinpol	3175.00		NIST Webbook
rinpol	3175.00		NIST Webbook
tb	1066.37	K	Joback Method
tc	1312.45	K	Joback Method
tf	598.54	K	Joback Method
vc	1.639	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1497.02	J/molxK	1066.37	Joback Method
cpg	1515.83	J/molxK	1107.38	Joback Method
cpg	1532.87	J/molxK	1148.40	Joback Method
cpg	1548.28	J/molxK	1189.41	Joback Method
cpg	1562.16	J/molxK	1230.42	Joback Method
cpg	1574.63	J/molxK	1271.44	Joback Method
cpg	1585.83	J/molxK	1312.45	Joback Method
dvisc	0.0001704	Paxs	598.54	Joback Method

dvisc	0.0000769	Paxs	676.51	Joback Method
dvisc	0.0000409	Paxs	754.48	Joback Method
dvisc	0.0000245	Paxs	832.45	Joback Method
dvisc	0.0000160	Paxs	910.43	Joback Method
dvisc	0.0000112	Paxs	988.40	Joback Method
dvisc	0.0000082	Paxs	1066.37	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=U377780&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377780&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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