

# Phthalic acid, pentadecyl trans-hex-3-enyl ester

Inchi:	InChI=1S/C29H46O4/c1-3-5-7-9-10-11-12-13-14-15-16-17-21-25-33-29(31)27-23-19-18-
InchiKey:	MXMVDZVYKLRZRW-SOFGYWHQSA-N
Formula:	C29H46O4
SMILES:	CCC=CCCOC(=O)c1cccc1C(=O)OCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	458.67

## Physical Properties

Property code	Value	Unit	Source
gf	-91.54	kJ/mol	Joback Method
hf	-789.21	kJ/mol	Joback Method
hfus	70.29	kJ/mol	Joback Method
hvap	101.36	kJ/mol	Joback Method
log10ws	-9.76		Crippen Method
logp	8.448		Crippen Method
mvol	406.290	ml/mol	McGowan Method
pc	797.08	kPa	Joback Method
rinpol	3246.00		NIST Webbook
rinpol	3246.00		NIST Webbook
tb	1051.32	K	Joback Method
tc	1293.56	K	Joback Method
tf	594.77	K	Joback Method
vc	1.579	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1404.37	J/molxK	1051.32	Joback Method
cpg	1422.82	J/molxK	1091.69	Joback Method
cpg	1439.62	J/molxK	1132.07	Joback Method
cpg	1454.85	J/molxK	1172.44	Joback Method
cpg	1468.62	J/molxK	1212.81	Joback Method
cpg	1481.02	J/molxK	1253.18	Joback Method
cpg	1492.17	J/molxK	1293.56	Joback Method
dvisc	0.0001929	Paxs	594.77	Joback Method

dvisc	0.0000946	Paxs	670.86	Joback Method
dvisc	0.0000537	Paxs	746.95	Joback Method
dvisc	0.0000338	Paxs	823.04	Joback Method
dvisc	0.0000230	Paxs	899.14	Joback Method
dvisc	0.0000166	Paxs	975.23	Joback Method
dvisc	0.0000126	Paxs	1051.32	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U360493&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U360493&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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