

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

Inchi:	InChI=1S/C34H58O4/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-23-26-37-32(35)30-
InchiKey:	YCWOUWJQUNXFGN-UHFFFAOYSA-N
Formula:	C34H58O4
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCC(C)CC(C)(C)C
Mol. weight [g/mol]:	530.82

## Physical Properties

Property code	Value	Unit	Source
gf	-129.26	kJ/mol	Joback Method
hf	-1023.66	kJ/mol	Joback Method
hfus	72.11	kJ/mol	Joback Method
hvap	110.84	kJ/mol	Joback Method
log10ws	-11.52		Crippen Method
logp	10.334		Crippen Method
mcvol	481.040	ml/mol	McGowan Method
pc	610.57	kPa	Joback Method
rinsol	3498.00		NIST Webbook
tb	1157.89	K	Joback Method
tc	1453.05	K	Joback Method
tf	643.62	K	Joback Method
vc	1.863	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1755.10	J/molxK	1157.89	Joback Method
cpg	1776.16	J/molxK	1207.08	Joback Method
cpg	1794.88	J/molxK	1256.28	Joback Method
cpg	1811.51	J/molxK	1305.47	Joback Method
cpg	1826.28	J/molxK	1354.66	Joback Method
cpg	1839.44	J/molxK	1403.86	Joback Method
cpg	1851.24	J/molxK	1453.05	Joback Method
dvisc	0.0000952	Paxs	643.62	Joback Method
dvisc	0.0000418	Paxs	729.33	Joback Method

dvisc	0.0000218	Paxs	815.04	Joback Method
dvisc	0.0000129	Paxs	900.75	Joback Method
dvisc	0.0000083	Paxs	986.47	Joback Method
dvisc	0.0000058	Paxs	1072.18	Joback Method
dvisc	0.0000042	Paxs	1157.89	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U377784&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377784&amp;Units=SI</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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