

# Phthalic acid, 4-methylhept-3-yl pentadecyl ester

Inchi:	InChI=1S/C31H52O4/c1-5-8-9-10-11-12-13-14-15-16-17-18-21-25-34-30(32)27-23-19-20
InchiKey:	FEDVQOKFLJAXHQ-UHFFFAOYSA-N
Formula:	C31H52O4
SMILES:	CCCCCCCCCCCCCOC(=O)c1cccc1C(=O)OC(CC)C(C)CCC
Mol. weight [g/mol]:	488.74

## Physical Properties

Property code	Value	Unit	Source
gf	-159.80	kJ/mol	Joback Method
hf	-958.27	kJ/mol	Joback Method
hfus	68.23	kJ/mol	Joback Method
hvap	105.07	kJ/mol	Joback Method
log10ws	-10.62		Crippen Method
logp	9.306		Crippen Method
mvol	438.770	ml/mol	McGowan Method
pc	703.59	kPa	Joback Method
rinpol	3301.00		NIST Webbook
rinpol	3301.00		NIST Webbook
tb	1092.04	K	Joback Method
tc	1353.20	K	Joback Method
tf	592.39	K	Joback Method
vc	1.700	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1561.07	J/molxK	1092.04	Joback Method
cpg	1634.32	J/molxK	1309.67	Joback Method
cpg	1623.70	J/molxK	1266.15	Joback Method
cpg	1611.18	J/molxK	1222.62	Joback Method
cpg	1596.64	J/molxK	1179.09	Joback Method
cpg	1579.98	J/molxK	1135.57	Joback Method
cpg	1643.16	J/molxK	1353.20	Joback Method
dvisc	0.0000086	Paxs	1092.04	Joback Method

dvisc	0.0000116	Paxs	1008.76	Joback Method
dvisc	0.0000166	Paxs	925.49	Joback Method
dvisc	0.0000256	Paxs	842.22	Joback Method
dvisc	0.0000432	Paxs	758.94	Joback Method
dvisc	0.0000831	Paxs	675.67	Joback Method
dvisc	0.0001919	Paxs	592.39	Joback Method

## Sources

<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=U377950&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377950&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

## Legend

<b>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>w<sub>s</sub>:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mc<sub>vol</sub>:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rin<sub>pol</sub>:</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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