

# Phthalic acid, 2-methylbenzyl pentadecyl ester

<b>Inchi:</b>	InChI=1S/C31H44O4/c1-3-4-5-6-7-8-9-10-11-12-13-14-19-24-34-30(32)28-22-17-18-23-2
<b>InchiKey:</b>	XYIYREHPOYJAQL-UHFFFAOYSA-N
<b>Formula:</b>	C31H44O4
<b>SMILES:</b>	CCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1ccccc1C
<b>Mol. weight [g/mol]:</b>	480.68

## Physical Properties

Property code	Value	Unit	Source
gf	-52.14	kJ/mol	Joback Method
hf	-722.65	kJ/mol	Joback Method
hfus	68.92	kJ/mol	Joback Method
hvap	108.79	kJ/mol	Joback Method
log10ws	-10.40		Crippen Method
logp	8.600		Crippen Method
mcvol	415.010	ml/mol	McGowan Method
pc	830.50	kPa	Joback Method
rinpol	3464.00		NIST Webbook
rinpol	3464.00		NIST Webbook
tb	1124.58	K	Joback Method
tc	1383.23	K	Joback Method
tf	661.33	K	Joback Method
vc	1.603	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1445.92	J/molxK	1124.58	Joback Method
cpg	1460.95	J/molxK	1167.69	Joback Method
cpg	1474.05	J/molxK	1210.80	Joback Method
cpg	1485.31	J/molxK	1253.90	Joback Method
cpg	1494.87	J/molxK	1297.01	Joback Method
cpg	1502.81	J/molxK	1340.12	Joback Method
cpg	1509.27	J/molxK	1383.23	Joback Method
dvisc	0.0001302	Paxs	661.33	Joback Method

dvisc	0.0000699	Paxs	738.54	Joback Method
dvisc	0.0000423	Paxs	815.75	Joback Method
dvisc	0.0000279	Paxs	892.95	Joback Method
dvisc	0.0000196	Paxs	970.16	Joback Method
dvisc	0.0000146	Paxs	1047.37	Joback Method
dvisc	0.0000113	Paxs	1124.58	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=U382861&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382861&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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