

# Phthalic acid, 2,4-dimethylpent-3-yl tridecyl ester

Inchi:	InChI=1S/C28H46O4/c1-6-7-8-9-10-11-12-13-14-15-18-21-31-27(29)24-19-16-17-20-25(
InchiKey:	IOKYJDBUNKIZCM-UHFFFAOYSA-N
Formula:	C28H46O4
SMILES:	CCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OC(C(C)C)C(C)C
Mol. weight [g/mol]:	446.66

## Physical Properties

Property code	Value	Unit	Source
gf	-187.50	kJ/mol	Joback Method
hf	-901.63	kJ/mol	Joback Method
hfus	56.93	kJ/mol	Joback Method
hvap	98.01	kJ/mol	Joback Method
log10ws	-9.12		Crippen Method
logp	7.992		Crippen Method
mcvol	396.500	ml/mol	McGowan Method
pc	828.59	kPa	Joback Method
rinpol	3004.00		NIST Webbook
tb	1022.96	K	Joback Method
tc	1254.27	K	Joback Method
tf	543.58	K	Joback Method
vc	1.526	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1370.42	J/molxK	1022.96	Joback Method
cpg	1388.20	J/molxK	1061.51	Joback Method
cpg	1404.20	J/molxK	1100.06	Joback Method
cpg	1418.49	J/molxK	1138.62	Joback Method
cpg	1431.14	J/molxK	1177.17	Joback Method
cpg	1442.20	J/molxK	1215.72	Joback Method
cpg	1451.76	J/molxK	1254.27	Joback Method
dvisc	0.0003269	Paxs	543.58	Joback Method
dvisc	0.0001341	Paxs	623.48	Joback Method

dvisc	0.0000674	Paxs	703.37	Joback Method
dvisc	0.0000389	Paxs	783.27	Joback Method
dvisc	0.0000249	Paxs	863.17	Joback Method
dvisc	0.0000172	Paxs	943.06	Joback Method
dvisc	0.0000126	Paxs	1022.96	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=U356852&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356852&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>

## 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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