

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

Inchi:	InChI=1S/C28H46O4/c1-6-8-9-10-11-12-13-14-15-16-19-22-31-26(29)23-20-17-18-21-24
InchiKey:	URMKTZPTSXJHG-UHFFFAOYSA-N
Formula:	C28H46O4
SMILES:	CCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OC(CC)C(C)(C)C
Mol. weight [g/mol]:	446.66

## Physical Properties

Property code	Value	Unit	Source
gf	-179.78	kJ/mol	Joback Method
hf	-899.82	kJ/mol	Joback Method
hfus	56.57	kJ/mol	Joback Method
hvap	97.49	kJ/mol	Joback Method
log10ws	-9.36		Crippen Method
logp	8.136		Crippen Method
mcvol	396.500	ml/mol	McGowan Method
pc	830.02	kPa	Joback Method
rinpol	2224.00		NIST Webbook
rinpol	2224.00		NIST Webbook
tb	1020.61	K	Joback Method
tc	1250.70	K	Joback Method
tf	576.00	K	Joback Method
vc	1.526	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1369.73	J/molxK	1020.61	Joback Method
cpg	1387.78	J/molxK	1058.96	Joback Method
cpg	1404.26	J/molxK	1097.31	Joback Method
cpg	1419.26	J/molxK	1135.65	Joback Method
cpg	1432.88	J/molxK	1174.00	Joback Method
cpg	1445.19	J/molxK	1212.35	Joback Method
cpg	1456.30	J/molxK	1250.70	Joback Method
dvisc	0.0002256	Paxs	576.00	Joback Method

dvisc	0.0001033	Paxs	650.10	Joback Method
dvisc	0.0000556	Paxs	724.20	Joback Method
dvisc	0.0000335	Paxs	798.31	Joback Method
dvisc	0.0000220	Paxs	872.41	Joback Method
dvisc	0.0000155	Paxs	946.51	Joback Method
dvisc	0.0000114	Paxs	1020.61	Joback Method

## Sources

<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=U415536&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U415536&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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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