

# Terephthalic acid, 2-methylpent-3-yl tetradecyl ester

Inchi:	InChI=1S/C28H46O4/c1-5-7-8-9-10-11-12-13-14-15-16-17-22-31-27(29)24-18-20-25(21-
InchiKey:	ZNZMXJGKTWERDF-UHFFFAOYSA-N
Formula:	C28H46O4
SMILES:	CCCCCCCCCCCCCOC(=O)c1ccc(C(=O)OC(CC)C(C)C)cc1
Mol. weight [g/mol]:	446.66

## Physical Properties

Property code	Value	Unit	Source
gf	-185.06	kJ/mol	Joback Method
hf	-896.35	kJ/mol	Joback Method
hfus	60.46	kJ/mol	Joback Method
hvap	98.40	kJ/mol	Joback Method
log10ws	-9.36		Crippen Method
logp	8.136		Crippen Method
mcvol	396.500	ml/mol	McGowan Method
pc	824.79	kPa	Joback Method
rinpol	3168.00		NIST Webbook
tb	1023.40	K	Joback Method
tc	1255.68	K	Joback Method
tf	558.58	K	Joback Method
vc	1.532	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1370.15	J/molxK	1023.40	Joback Method
cpg	1388.07	J/molxK	1062.11	Joback Method
cpg	1404.21	J/molxK	1100.83	Joback Method
cpg	1418.64	J/molxK	1139.54	Joback Method
cpg	1431.44	J/molxK	1178.25	Joback Method
cpg	1442.65	J/molxK	1216.97	Joback Method
cpg	1452.37	J/molxK	1255.68	Joback Method
dvisc	0.0002898	Paxs	558.58	Joback Method
dvisc	0.0001282	Paxs	636.05	Joback Method

dvisc	0.0000677	Paxs	713.52	Joback Method
dvisc	0.0000405	Paxs	790.99	Joback Method
dvisc	0.0000266	Paxs	868.46	Joback Method
dvisc	0.0000187	Paxs	945.93	Joback Method
dvisc	0.0000138	Paxs	1023.40	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U356205&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356205&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>
<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>

## 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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