

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

<b>Inchi:</b>	InChI=1S/C29H48O4/c1-5-7-8-9-10-11-12-13-14-15-16-17-18-23-32-28(30)25-19-21-26(
<b>InchiKey:</b>	WBOBVJMLLCFPSM-UHFFFAOYSA-N
<b>Formula:</b>	C29H48O4
<b>SMILES:</b>	CCCCCCCCCCCCCOC(=O)c1ccc(C(=O)OC(CC)C(C)C)cc1
<b>Mol. weight [g/mol]:</b>	460.69

## Physical Properties

Property code	Value	Unit	Source
gf	-176.64	kJ/mol	Joback Method
hf	-916.99	kJ/mol	Joback Method
hfus	63.05	kJ/mol	Joback Method
hvap	100.62	kJ/mol	Joback Method
log10ws	-9.78		Crippen Method
logp	8.526		Crippen Method
mvol	410.590	ml/mol	McGowan Method
pc	781.12	kPa	Joback Method
rinpol	3272.00		NIST Webbook
rinpol	3272.00		NIST Webbook
tb	1046.28	K	Joback Method
tc	1286.84	K	Joback Method
tf	569.85	K	Joback Method
vc	1.587	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1433.52	J/molxK	1046.28	Joback Method
cpg	1451.74	J/molxK	1086.37	Joback Method
cpg	1468.04	J/molxK	1126.47	Joback Method
cpg	1482.52	J/molxK	1166.56	Joback Method
cpg	1495.24	J/molxK	1206.65	Joback Method
cpg	1506.29	J/molxK	1246.75	Joback Method
cpg	1515.75	J/molxK	1286.84	Joback Method
dvisc	0.0002531	Paxs	569.85	Joback Method

dvisc	0.0001111	Paxs	649.25	Joback Method
dvisc	0.0000584	Paxs	728.66	Joback Method
dvisc	0.0000348	Paxs	808.06	Joback Method
dvisc	0.0000228	Paxs	887.47	Joback Method
dvisc	0.0000160	Paxs	966.88	Joback Method
dvisc	0.0000118	Paxs	1046.28	Joback Method

## Sources

<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=U356206&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356206&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

## 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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