

# Terephthalic acid, heptadecyl hept-3-yl ester

<b>Other names:</b>	Terephthalic acid, heptadecyl heptyl-3 ester
<b>Inchi:</b>	InChI=1S/C32H54O4/c1-4-7-9-10-11-12-13-14-15-16-17-18-19-20-21-27-35-31(33)28-23
<b>InchiKey:</b>	PWZTVEDHBBEOKX-UHFFFAOYSA-N
<b>Formula:</b>	C32H54O4
<b>SMILES:</b>	CCCCCCCCCCCCCCCCOC(=O)c1ccc(C(=O)OC(CC)CCCC)cc1
<b>Mol. weight [g/mol]:</b>	502.77

## Physical Properties

Property code	Value	Unit	Source
gf	-148.94	kJ/mol	Joback Method
hf	-973.63	kJ/mol	Joback Method
hfus	74.34	kJ/mol	Joback Method
hvap	107.69	kJ/mol	Joback Method
log10ws	-11.28		Crippen Method
logp	9.840		Crippen Method
mvol	452.860	ml/mol	McGowan Method
pc	666.32	kPa	Joback Method
rinpol	3602.00		NIST Webbook
tb	1115.36	K	Joback Method
tc	1392.23	K	Joback Method
tf	618.66	K	Joback Method
vc	1.762	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1625.12	J/molxK	1115.36	Joback Method
cpg	1644.77	J/molxK	1161.51	Joback Method
cpg	1661.93	J/molxK	1207.65	Joback Method
cpg	1676.76	J/molxK	1253.80	Joback Method
cpg	1689.40	J/molxK	1299.94	Joback Method
cpg	1699.99	J/molxK	1346.09	Joback Method
cpg	1708.67	J/molxK	1392.23	Joback Method
dvisc	0.0001518	Paxs	618.66	Joback Method

dvisc	0.0000697	Paxs	701.44	Joback Method
dvisc	0.0000377	Paxs	784.23	Joback Method
dvisc	0.0000230	Paxs	867.01	Joback Method
dvisc	0.0000152	Paxs	949.79	Joback Method
dvisc	0.0000108	Paxs	1032.58	Joback Method
dvisc	0.0000081	Paxs	1115.36	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=U356652&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356652&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>

## 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

Latest version available from:

<https://www.chemeo.com/cid/56-593-2/Terephthalic-acid-heptadecyl-hept-3-yl-ester.pdf>

Generated by Cheméo on 2024-04-19 19:24:13.341231006 +0000 UTC m=+15843902.261808340.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.