

# Terephthalic acid, but-2-enyl hexadecyl ester

**Inchi:** InChI=1S/C28H44O4/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-24-32-28(30)26-21-19-2  
**InchiKey:** JEICTQRAGOXXKN-GQCTYLIASA-N  
**Formula:** C28H44O4  
**SMILES:** CC=CCOC(=O)c1ccc(C(=O)OCCCCCCCCCCCCCCCC)cc1  
**Mol. weight [g/mol]:** 444.65

## Physical Properties

Property code	Value	Unit	Source
gf	-99.96	kJ/mol	Joback Method
hf	-768.57	kJ/mol	Joback Method
hfus	67.70	kJ/mol	Joback Method
hvap	99.13	kJ/mol	Joback Method
log10ws	-9.34		Crippen Method
logp	8.058		Crippen Method
mcvol	392.200	ml/mol	McGowan Method
pc	842.11	kPa	Joback Method
rinpol	3427.00		NIST Webbook
tb	1028.44	K	Joback Method
tc	1262.21	K	Joback Method
tf	583.50	K	Joback Method
vc	1.524	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1340.94	J/molxK	1028.44	Joback Method
cpg	1358.94	J/molxK	1067.40	Joback Method
cpg	1375.39	J/molxK	1106.36	Joback Method
cpg	1390.37	J/molxK	1145.33	Joback Method
cpg	1403.97	J/molxK	1184.29	Joback Method
cpg	1416.27	J/molxK	1223.25	Joback Method
cpg	1427.36	J/molxK	1262.21	Joback Method
dvisc	0.0002193	Paxs	583.50	Joback Method
dvisc	0.0001085	Paxs	657.66	Joback Method

dvisc	0.0000619	Paxs	731.81	Joback Method
dvisc	0.0000392	Paxs	805.97	Joback Method
dvisc	0.0000268	Paxs	880.13	Joback Method
dvisc	0.0000194	Paxs	954.28	Joback Method
dvisc	0.0000147	Paxs	1028.44	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=U356324&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356324&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>

## 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/11-058-5/Terephthalic-acid-but-2-enyl-hexadecyl-ester.pdf>

Generated by Cheméo on 2024-04-29 01:37:03.486244346 +0000 UTC m=+16643872.406821657.

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