

# Terephthalic acid, 4-heptyl hexadecyl ester

**Inchi:** InChI=1S/C31H52O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-26-34-30(32)27-22-24-  
**InchiKey:** OWQPXRWBMBXONR-UHFFFAOYSA-N  
**Formula:** C31H52O4  
**SMILES:** CCCCCCCCCCCCCCOC(=O)c1ccc(C(=O)OC(CCC)CCC)cc1  
**Mol. weight [g/mol]:** 488.74

## Physical Properties

Property code	Value	Unit	Source
gf	-157.36	kJ/mol	Joback Method
hf	-952.99	kJ/mol	Joback Method
hfus	71.75	kJ/mol	Joback Method
hvap	105.46	kJ/mol	Joback Method
log10ws	-10.86		Crippen Method
logp	9.450		Crippen Method
mcvol	438.770	ml/mol	McGowan Method
pc	700.61	kPa	Joback Method
rinpol	3465.00		NIST Webbook
tb	1092.48	K	Joback Method
tc	1356.26	K	Joback Method
tf	607.39	K	Joback Method
vc	1.706	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1560.96	J/molxK	1092.48	Joback Method
cpg	1580.15	J/molxK	1136.44	Joback Method
cpg	1597.09	J/molxK	1180.41	Joback Method
cpg	1611.87	J/molxK	1224.37	Joback Method
cpg	1624.62	J/molxK	1268.34	Joback Method
cpg	1635.46	J/molxK	1312.30	Joback Method
cpg	1644.50	J/molxK	1356.26	Joback Method
dvisc	0.0001743	Paxs	607.39	Joback Method
dvisc	0.0000806	Paxs	688.24	Joback Method

dvisc	0.0000439	Paxs	769.09	Joback Method
dvisc	0.0000268	Paxs	849.93	Joback Method
dvisc	0.0000178	Paxs	930.78	Joback Method
dvisc	0.0000127	Paxs	1011.63	Joback Method
dvisc	0.0000095	Paxs	1092.48	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U356166&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356166&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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