

# Terephthalic acid, 3-methylbutyl tridecyl ester

<b>Inchi:</b>	InChI=1S/C26H42O4/c1-4-5-6-7-8-9-10-11-12-13-14-20-29-25(27)23-15-17-24(18-16-23
<b>InchiKey:</b>	VPDAYXOUERWLNC-UHFFFAOYSA-N
<b>Formula:</b>	C26H42O4
<b>SMILES:</b>	CCCCCCCCCCCCOC(=O)c1ccc(C(=O)OCCC(C)C)cc1
<b>Mol. weight [g/mol]:</b>	418.61

## Physical Properties

Property code	Value	Unit	Source
gf	-199.46	kJ/mol	Joback Method
hf	-849.79	kJ/mol	Joback Method
hfus	58.80	kJ/mol	Joback Method
hvap	94.33	kJ/mol	Joback Method
log10ws	-8.41		Crippen Method
logp	7.357		Crippen Method
mcvol	368.320	ml/mol	McGowan Method
pc	919.39	kPa	Joback Method
rinpol	3064.00		NIST Webbook
tb	978.08	K	Joback Method
tc	1197.65	K	Joback Method
tf	551.04	K	Joback Method
vc	1.425	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1244.04	J/molxK	978.08	Joback Method
cpg	1261.53	J/molxK	1014.67	Joback Method
cpg	1277.47	J/molxK	1051.27	Joback Method
cpg	1291.91	J/molxK	1087.86	Joback Method
cpg	1304.90	J/molxK	1124.46	Joback Method
cpg	1316.49	J/molxK	1161.05	Joback Method
cpg	1326.73	J/molxK	1197.65	Joback Method
dvisc	0.0003362	Paxs	551.04	Joback Method
dvisc	0.0001620	Paxs	622.21	Joback Method

dvisc	0.0000907	Paxs	693.39	Joback Method
dvisc	0.0000566	Paxs	764.56	Joback Method
dvisc	0.0000383	Paxs	835.73	Joback Method
dvisc	0.0000275	Paxs	906.91	Joback Method
dvisc	0.0000207	Paxs	978.08	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=U356145&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356145&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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/23-229-2/Terephthalic-acid-3-methylbutyl-tridecyl-ester.pdf>

Generated by Cheméo on 2024-04-20 15:20:13.99762475 +0000 UTC m=+15915662.918202062.

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