

# Terephthalic acid, but-3-enyl tetradecyl ester

<b>Inchi:</b>	InChI=1S/C26H40O4/c1-3-5-7-8-9-10-11-12-13-14-15-16-22-30-26(28)24-19-17-23(18-2
<b>InchiKey:</b>	UDJUTGZTMZZFSI-UHFFFAOYSA-N
<b>Formula:</b>	C26H40O4
<b>SMILES:</b>	C=CCCOC(=O)c1ccc(C(=O)OCCCCCCCCCCCCC)cc1
<b>Mol. weight [g/mol]:</b>	416.59

## Physical Properties

Property code	Value	Unit	Source
gf	-109.18	kJ/mol	Joback Method
hf	-719.08	kJ/mol	Joback Method
hfus	61.04	kJ/mol	Joback Method
hvap	94.05	kJ/mol	Joback Method
log10ws	-8.51		Crippen Method
logp	7.277		Crippen Method
mcvol	364.020	ml/mol	McGowan Method
pc	938.64	kPa	Joback Method
rinsol	3181.00		NIST Webbook
tb	975.20	K	Joback Method
tc	1194.07	K	Joback Method
tf	564.28	K	Joback Method
vc	1.413	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1213.85	J/molxK	975.20	Joback Method
cpg	1285.48	J/molxK	1157.59	Joback Method
cpg	1273.85	J/molxK	1121.12	Joback Method
cpg	1260.92	J/molxK	1084.64	Joback Method
cpg	1246.65	J/molxK	1048.16	Joback Method
cpg	1230.98	J/molxK	1011.68	Joback Method
cpg	1295.89	J/molxK	1194.07	Joback Method
dvisc	0.0000246	Paxs	975.20	Joback Method
dvisc	0.0000321	Paxs	906.71	Joback Method

dvisc	0.0000436	Paxs	838.23	Joback Method
dvisc	0.0000626	Paxs	769.74	Joback Method
dvisc	0.0000966	Paxs	701.25	Joback Method
dvisc	0.0001635	Paxs	632.77	Joback Method
dvisc	0.0003147	Paxs	564.28	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=U356344&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356344&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

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