

# Terephthalic acid, but-3-enyl octyl ester

**Inchi:** InChI=1S/C20H28O4/c1-3-5-7-8-9-10-16-24-20(22)18-13-11-17(12-14-18)19(21)23-15-6  
**InchiKey:** ASKVHHFSVZHKLR-UHFFFAOYSA-N  
**Formula:** C20H28O4  
**SMILES:** C=CCCOC(=O)c1ccc(C(=O)OCCCCCCCC)cc1  
**Mol. weight [g/mol]:** 332.43

## Physical Properties

Property code	Value	Unit	Source
gf	-159.70	kJ/mol	Joback Method
hf	-595.24	kJ/mol	Joback Method
hfus	45.50	kJ/mol	Joback Method
hvap	80.69	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	4.937		Crippen Method
mcvol	279.480	ml/mol	McGowan Method
pc	1384.02	kPa	Joback Method
rinpol	2543.00		NIST Webbook
tb	837.92	K	Joback Method
tc	1039.38	K	Joback Method
tf	496.66	K	Joback Method
vc	1.077	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	850.45	J/molxK	837.92	Joback Method
cpg	918.01	J/molxK	1005.80	Joback Method
cpg	906.58	J/molxK	972.22	Joback Method
cpg	894.14	J/molxK	938.65	Joback Method
cpg	880.65	J/molxK	905.07	Joback Method
cpg	866.10	J/molxK	871.50	Joback Method
cpg	928.45	J/molxK	1039.38	Joback Method
dvisc	0.0000586	Paxs	837.92	Joback Method
dvisc	0.0000751	Paxs	781.04	Joback Method

dvisc	0.0000999	Paxs	724.17	Joback Method
dvisc	0.0001397	Paxs	667.29	Joback Method
dvisc	0.0002080	Paxs	610.41	Joback Method
dvisc	0.0003358	Paxs	553.54	Joback Method
dvisc	0.0006053	Paxs	496.66	Joback Method

## Sources

<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=U356338&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356338&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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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