

# Terephthalic acid, but-2-enyl isobutyl ester

<b>Inchi:</b>	InChI=1S/C16H20O4/c1-4-5-10-19-15(17)13-6-8-14(9-7-13)16(18)20-11-12(2)3/h4-9,12H
<b>InchiKey:</b>	MGGGGDZVIFIYRK-SNAWJCMRSA-N
<b>Formula:</b>	C16H20O4
<b>SMILES:</b>	CC=CCOC(=O)c1ccc(C(=O)OCC(C)C)cc1
<b>Mol. weight [g/mol]:</b>	276.33

## Physical Properties

Property code	Value	Unit	Source
gf	-203.44	kJ/mol	Joback Method
hf	-526.17	kJ/mol	Joback Method
hfus	33.10	kJ/mol	Joback Method
hvap	72.03	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	3.232		Crippen Method
mcvol	223.120	ml/mol	McGowan Method
pc	1913.58	kPa	Joback Method
rinpol	2147.00		NIST Webbook
tb	753.44	K	Joback Method
tc	964.70	K	Joback Method
tf	433.26	K	Joback Method
vc	0.846	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	624.51	J/molxK	753.44	Joback Method
cpg	639.34	J/molxK	788.65	Joback Method
cpg	653.17	J/molxK	823.86	Joback Method
cpg	666.02	J/molxK	859.07	Joback Method
cpg	677.92	J/molxK	894.28	Joback Method
cpg	688.90	J/molxK	929.49	Joback Method
cpg	698.98	J/molxK	964.70	Joback Method
dvisc	0.0009089	Paxs	433.26	Joback Method
dvisc	0.0004767	Paxs	486.62	Joback Method

dvisc	0.0002840	Paxs	539.99	Joback Method
dvisc	0.0001857	Paxs	593.35	Joback Method
dvisc	0.0001303	Paxs	646.71	Joback Method
dvisc	0.0000965	Paxs	700.08	Joback Method
dvisc	0.0000745	Paxs	753.44	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=U356311&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356311&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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