

# Terephthalic acid, ethyl 5-methylhex-2-yl ester

<b>Inchi:</b>	InChI=1S/C17H24O4/c1-5-20-16(18)14-8-10-15(11-9-14)17(19)21-13(4)7-6-12(2)3/h8-13
<b>InchiKey:</b>	XYZMPNBHVXJIGO-UHFFFAOYSA-N
<b>Formula:</b>	C17H24O4
<b>SMILES:</b>	CCOC(=O)c1ccc(C(=O)OC(C)CCC(C)C)cc1
<b>Mol. weight [g/mol]:</b>	292.37

## Physical Properties

Property code	Value	Unit	Source
gf	-277.68	kJ/mol	Joback Method
hf	-669.31	kJ/mol	Joback Method
hfus	31.97	kJ/mol	Joback Method
hvap	73.91	kJ/mol	Joback Method
log10ws	-4.76		Crippen Method
logp	3.845		Crippen Method
mvol	241.510	ml/mol	McGowan Method
pc	1699.10	kPa	Joback Method
rinpol	2348.00		NIST Webbook
rinpol	2348.00		NIST Webbook
tb	771.72	K	Joback Method
tc	977.62	K	Joback Method
tf	434.61	K	Joback Method
vc	0.915	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	705.43	J/molxK	771.72	Joback Method
cpg	721.28	J/molxK	806.04	Joback Method
cpg	736.04	J/molxK	840.35	Joback Method
cpg	749.74	J/molxK	874.67	Joback Method
cpg	762.38	J/molxK	908.99	Joback Method
cpg	773.98	J/molxK	943.31	Joback Method
cpg	784.57	J/molxK	977.62	Joback Method
dvisc	0.0010554	Paxs	434.61	Joback Method

dvisc	0.0005175	Paxs	490.80	Joback Method
dvisc	0.0002938	Paxs	546.98	Joback Method
dvisc	0.0001853	Paxs	603.16	Joback Method
dvisc	0.0001265	Paxs	659.35	Joback Method
dvisc	0.0000916	Paxs	715.54	Joback Method
dvisc	0.0000696	Paxs	771.72	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=U382994&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382994&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>

## Legend

<b>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>w<sub>s</sub>:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mc<sub>vol</sub>:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rin<sub>pol</sub>:</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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