

# Phthalic acid, 2,4-dimethylpent-3-yl ethyl ester

<b>Inchi:</b>	InChI=1S/C17H24O4/c1-6-20-16(18)13-9-7-8-10-14(13)17(19)21-15(11(2)3)12(4)5/h7-12
<b>InchiKey:</b>	XLDNTVLUZTWLER-UHFFFAOYSA-N
<b>Formula:</b>	C17H24O4
<b>SMILES:</b>	CCOC(=O)c1cccc1C(=O)OC(C(C)C)C(C)C
<b>Mol. weight [g/mol]:</b>	292.37

## Physical Properties

Property code	Value	Unit	Source
gf	-280.12	kJ/mol	Joback Method
hf	-674.59	kJ/mol	Joback Method
hfus	28.44	kJ/mol	Joback Method
hvap	73.52	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	3.701		Crippen Method
mvol	241.510	ml/mol	McGowan Method
pc	1710.36	kPa	Joback Method
rinpol	1927.00		NIST Webbook
rinpol	1927.00		NIST Webbook
tb	771.28	K	Joback Method
tc	980.14	K	Joback Method
tf	419.61	K	Joback Method
vc	0.909	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	705.98	J/molxK	771.28	Joback Method
cpg	722.05	J/molxK	806.09	Joback Method
cpg	737.00	J/molxK	840.90	Joback Method
cpg	750.84	J/molxK	875.71	Joback Method
cpg	763.59	J/molxK	910.52	Joback Method
cpg	775.27	J/molxK	945.33	Joback Method
cpg	785.88	J/molxK	980.14	Joback Method
dvisc	0.0012619	Paxs	419.61	Joback Method

dvisc	0.0005663	Paxs	478.22	Joback Method
dvisc	0.0003027	Paxs	536.83	Joback Method
dvisc	0.0001830	Paxs	595.45	Joback Method
dvisc	0.0001211	Paxs	654.06	Joback Method
dvisc	0.0000858	Paxs	712.67	Joback Method
dvisc	0.0000640	Paxs	771.28	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U356841&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356841&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>
<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>

## 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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