

# Phthalic acid, ethyl 4-methylhept-3-yl ester

**Inchi:** InChI=1S/C18H26O4/c1-5-10-13(4)16(6-2)22-18(20)15-12-9-8-11-14(15)17(19)21-7-3/h8  
**InchiKey:** KQBLOTIFIHRUBV-UHFFFAOYSA-N  
**Formula:** C18H26O4  
**SMILES:** CCCC(C)C(CC)OC(=O)c1ccccc1C(=O)OCC  
**Mol. weight [g/mol]:** 306.40

## Physical Properties

Property code	Value	Unit	Source
gf	-269.26	kJ/mol	Joback Method
hf	-689.95	kJ/mol	Joback Method
hfus	34.56	kJ/mol	Joback Method
hvap	76.14	kJ/mol	Joback Method
log10ws	-5.18		Crippen Method
logp	4.235		Crippen Method
mcvol	255.600	ml/mol	McGowan Method
pc	1572.21	kPa	Joback Method
rinpol	2002.00		NIST Webbook
tb	794.60	K	Joback Method
tc	999.14	K	Joback Method
tf	445.88	K	Joback Method
vc	0.972	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.32	J/mol×K	794.60	Joback Method
cpg	778.37	J/mol×K	828.69	Joback Method
cpg	793.31	J/mol×K	862.78	Joback Method
cpg	807.15	J/mol×K	896.87	Joback Method
cpg	819.91	J/mol×K	930.96	Joback Method
cpg	831.61	J/mol×K	965.05	Joback Method
cpg	842.26	J/mol×K	999.14	Joback Method
dvisc	0.0009566	Paxs	445.88	Joback Method
dvisc	0.0004637	Paxs	504.00	Joback Method

dvisc	0.0002611	Paxs	562.12	Joback Method
dvisc	0.0001637	Paxs	620.24	Joback Method
dvisc	0.0001112	Paxs	678.36	Joback Method
dvisc	0.0000803	Paxs	736.48	Joback Method
dvisc	0.0000608	Paxs	794.60	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=U377936&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377936&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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