

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

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

## Physical Properties

Property code	Value	Unit	Source
gf	-271.70	kJ/mol	Joback Method
hf	-695.23	kJ/mol	Joback Method
hfus	31.03	kJ/mol	Joback Method
hvap	75.75	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.091		Crippen Method
mcvol	255.600	ml/mol	McGowan Method
pc	1582.23	kPa	Joback Method
rinsol	2015.00		NIST Webbook
tb	794.16	K	Joback Method
tc	1001.35	K	Joback Method
tf	430.88	K	Joback Method
vc	0.966	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.86	J/molxK	794.16	Joback Method
cpg	779.12	J/molxK	828.69	Joback Method
cpg	794.22	J/molxK	863.22	Joback Method
cpg	808.19	J/molxK	897.75	Joback Method
cpg	821.04	J/molxK	932.29	Joback Method
cpg	832.78	J/molxK	966.82	Joback Method
cpg	843.45	J/molxK	1001.35	Joback Method
dvisc	0.0011366	Paxs	430.88	Joback Method
dvisc	0.0005049	Paxs	491.43	Joback Method

dvisc	0.0002680	Paxs	551.97	Joback Method
dvisc	0.0001612	Paxs	612.52	Joback Method
dvisc	0.0001063	Paxs	673.07	Joback Method
dvisc	0.0000751	Paxs	733.61	Joback Method
dvisc	0.0000559	Paxs	794.16	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U356842&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356842&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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