

# Phthalic acid, heptyl hept-4-yl ester

**Inchi:** InChI=1S/C22H34O4/c1-4-7-8-9-12-17-25-21(23)19-15-10-11-16-20(19)22(24)26-18(13-  
**InchiKey:** ZMSMNYFFCDXGAR-UHFFFAOYSA-N  
**Formula:** C22H34O4  
**SMILES:** CCCCCCOC(=O)c1cccc1C(=O)OC(CCC)CCC  
**Mol. weight [g/mol]:** 362.50

## Physical Properties

Property code	Value	Unit	Source
gf	-233.14	kJ/mol	Joback Method
hf	-767.23	kJ/mol	Joback Method
hfus	48.44	kJ/mol	Joback Method
hvap	85.43	kJ/mol	Joback Method
log10ws	-7.09		Crippen Method
logp	5.939		Crippen Method
mvol	311.960	ml/mol	McGowan Method
pc	1177.66	kPa	Joback Method
rinpol	2420.00		NIST Webbook
rinpol	2420.00		NIST Webbook
tb	886.56	K	Joback Method
tc	1090.83	K	Joback Method
tf	505.96	K	Joback Method
vc	1.202	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.77	J/molxK	886.56	Joback Method
cpg	1014.40	J/molxK	920.61	Joback Method
cpg	1029.77	J/molxK	954.65	Joback Method
cpg	1043.91	J/molxK	988.70	Joback Method
cpg	1056.86	J/molxK	1022.74	Joback Method
cpg	1068.64	J/molxK	1056.79	Joback Method
cpg	1079.28	J/molxK	1090.83	Joback Method
dvisc	0.0005411	Paxs	505.96	Joback Method

dvisc	0.0002711	Paxs	569.39	Joback Method
dvisc	0.0001560	Paxs	632.83	Joback Method
dvisc	0.0000993	Paxs	696.26	Joback Method
dvisc	0.0000682	Paxs	759.69	Joback Method
dvisc	0.0000496	Paxs	823.13	Joback Method
dvisc	0.0000377	Paxs	886.56	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U356788&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356788&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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