

# Phthalic acid, hept-3-yl hexyl ester

<b>Inchi:</b>	InChI=1S/C21H32O4/c1-4-7-9-12-16-24-20(22)18-14-10-11-15-19(18)21(23)25-17(6-3)1
<b>InchiKey:</b>	RETDYOUXAYFAMO-UHFFFAOYSA-N
<b>Formula:</b>	C21H32O4
<b>SMILES:</b>	CCCCCOC(=O)c1ccccc1C(=O)OC(CC)CCCC
<b>Mol. weight [g/mol]:</b>	348.48

## Physical Properties

Property code	Value	Unit	Source
gf	-241.56	kJ/mol	Joback Method
hf	-746.59	kJ/mol	Joback Method
hfus	45.85	kJ/mol	Joback Method
hvap	83.20	kJ/mol	Joback Method
log10ws	-6.67		Crippen Method
logp	5.549		Crippen Method
mcvol	297.870	ml/mol	McGowan Method
pc	1259.27	kPa	Joback Method
rinsol	2342.00		NIST Webbook
tb	863.68	K	Joback Method
tc	1066.32	K	Joback Method
tf	494.69	K	Joback Method
vc	1.145	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	937.65	J/mol×K	863.68	Joback Method
cpg	954.09	J/mol×K	897.45	Joback Method
cpg	969.33	J/mol×K	931.23	Joback Method
cpg	983.39	J/mol×K	965.00	Joback Method
cpg	996.30	J/mol×K	998.77	Joback Method
cpg	1008.08	J/mol×K	1032.54	Joback Method
cpg	1018.76	J/mol×K	1066.32	Joback Method
dvisc	0.0006043	Paxs	494.69	Joback Method
dvisc	0.0003060	Paxs	556.19	Joback Method

dvisc	0.0001775	Paxs	617.69	Joback Method
dvisc	0.0001136	Paxs	679.18	Joback Method
dvisc	0.0000783	Paxs	740.68	Joback Method
dvisc	0.0000571	Paxs	802.18	Joback Method
dvisc	0.0000436	Paxs	863.68	Joback Method

## Sources

<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=U356990&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356990&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>

## 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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