

# Phthalic acid, heptyl 2-methylpent-3-yl ester

<b>Inchi:</b>	InChI=1S/C21H32O4/c1-5-7-8-9-12-15-24-20(22)17-13-10-11-14-18(17)21(23)25-19(6-2
<b>InchiKey:</b>	GQYKIKUZBPDBSP-UHFFFAOYSA-N
<b>Formula:</b>	C21H32O4
<b>SMILES:</b>	CCCCCCCOC(=O)c1ccccc1C(=O)OC(CC)C(C)C
<b>Mol. weight [g/mol]:</b>	348.48

## Physical Properties

Property code	Value	Unit	Source
gf	-244.00	kJ/mol	Joback Method
hf	-751.87	kJ/mol	Joback Method
hfus	42.33	kJ/mol	Joback Method
hvap	82.81	kJ/mol	Joback Method
log10ws	-6.43		Crippen Method
logp	5.405		Crippen Method
mcvol	297.870	ml/mol	McGowan Method
pc	1266.45	kPa	Joback Method
rinsol	2348.00		NIST Webbook
tb	863.24	K	Joback Method
tc	1067.43	K	Joback Method
tf	479.69	K	Joback Method
vc	1.139	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	938.15	J/molxK	863.24	Joback Method
cpg	1008.83	J/molxK	1033.40	Joback Method
cpg	997.06	J/molxK	999.37	Joback Method
cpg	984.13	J/molxK	965.34	Joback Method
cpg	970.02	J/molxK	931.30	Joback Method
cpg	954.70	J/molxK	897.27	Joback Method
cpg	1019.48	J/molxK	1067.43	Joback Method
dvisc	0.0000399	Paxs	863.24	Joback Method
dvisc	0.0000531	Paxs	799.32	Joback Method

dvisc	0.0000742	Paxs	735.39	Joback Method
dvisc	0.0001106	Paxs	671.47	Joback Method
dvisc	0.0001793	Paxs	607.54	Joback Method
dvisc	0.0003257	Paxs	543.62	Joback Method
dvisc	0.0006933	Paxs	479.69	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U356912&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356912&amp;Units=SI</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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