

# Isophthalic acid, oct-3-en-2-yl pentyl ester

<b>Inchi:</b>	InChI=1S/C21H30O4/c1-4-6-8-9-12-17(3)25-21(23)19-14-11-13-18(16-19)20(22)24-15-1
<b>InchiKey:</b>	SIUBVVWVGUIHFX-FMIVXFBMSA-N
<b>Formula:</b>	C21H30O4
<b>SMILES:</b>	CCCCC=CC(C)OC(=O)c1cccc(C(=O)OCCCC)c1
<b>Mol. weight [g/mol]:</b>	346.46

## Physical Properties

Property code	Value	Unit	Source
gf	-161.34	kJ/mol	Joback Method
hf	-629.37	kJ/mol	Joback Method
hfus	46.05	kJ/mol	Joback Method
hvap	83.16	kJ/mol	Joback Method
log10ws	-6.53		Crippen Method
logp	5.325		Crippen Method
mcvol	293.570	ml/mol	McGowan Method
pc	1307.06	kPa	Joback Method
rinpol	2530.00		NIST Webbook
rinpol	2530.00		NIST Webbook
tb	867.84	K	Joback Method
tc	1074.27	K	Joback Method
tf	489.61	K	Joback Method
vc	1.125	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	910.79	J/molxK	867.84	Joback Method
cpg	979.79	J/molxK	1039.87	Joback Method
cpg	968.11	J/molxK	1005.46	Joback Method
cpg	955.41	J/molxK	971.06	Joback Method
cpg	941.65	J/molxK	936.65	Joback Method
cpg	926.79	J/molxK	902.25	Joback Method
cpg	990.48	J/molxK	1074.27	Joback Method
dvisc	0.0000380	Paxs	867.84	Joback Method

dvisc	0.0000500	Paxs	804.80	Joback Method
dvisc	0.0000687	Paxs	741.76	Joback Method
dvisc	0.0001004	Paxs	678.72	Joback Method
dvisc	0.0001583	Paxs	615.69	Joback Method
dvisc	0.0002770	Paxs	552.65	Joback Method
dvisc	0.0005598	Paxs	489.61	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U343893&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U343893&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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