

# Isophthalic acid, pentyl undec-2-en-1-yl ester

<b>Inchi:</b>	InChI=1S/C24H36O4/c1-3-5-7-8-9-10-11-12-14-19-28-24(26)22-17-15-16-21(20-22)23(2
<b>InchiKey:</b>	MDIBTHBUUIQCED-WYMLVPIESA-N
<b>Formula:</b>	C24H36O4
<b>SMILES:</b>	CCCCCCCC=CCOC(=O)c1cccc(C(=O)OCCCC)c1
<b>Mol. weight [g/mol]:</b>	388.54

## Physical Properties

Property code	Value	Unit	Source
gf	-133.64	kJ/mol	Joback Method
hf	-686.01	kJ/mol	Joback Method
hfus	57.34	kJ/mol	Joback Method
hvap	90.23	kJ/mol	Joback Method
log10ws	-7.67		Crippen Method
logp	6.497		Crippen Method
mvol	335.840	ml/mol	McGowan Method
pc	1066.57	kPa	Joback Method
rinpol	2954.00		NIST Webbook
rinpol	2954.00		NIST Webbook
tb	936.92	K	Joback Method
tc	1148.38	K	Joback Method
tf	538.42	K	Joback Method
vc	1.300	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1091.52	J/molxK	936.92	Joback Method
cpg	1108.15	J/molxK	972.16	Joback Method
cpg	1123.53	J/molxK	1007.41	Joback Method
cpg	1137.72	J/molxK	1042.65	Joback Method
cpg	1150.76	J/molxK	1077.89	Joback Method
cpg	1162.71	J/molxK	1113.14	Joback Method
cpg	1173.61	J/molxK	1148.38	Joback Method
dvisc	0.0003558	Paxs	538.42	Joback Method

dvisc	0.0001828	Paxs	604.84	Joback Method
dvisc	0.0001072	Paxs	671.25	Joback Method
dvisc	0.0000692	Paxs	737.67	Joback Method
dvisc	0.0000480	Paxs	804.09	Joback Method
dvisc	0.0000352	Paxs	870.50	Joback Method
dvisc	0.0000270	Paxs	936.92	Joback Method

## Sources

<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=U343906&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U343906&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>

## 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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