

# Isophthalic acid, heptyl trans-hex-3-enyl ester

<b>Inchi:</b>	InChI=1S/C21H30O4/c1-3-5-7-9-11-16-25-21(23)19-14-12-13-18(17-19)20(22)24-15-10-
<b>InchiKey:</b>	JSUXCRKEYWSBRB-SOFGYWHQSA-N
<b>Formula:</b>	C21H30O4
<b>SMILES:</b>	CCC=CCCOC(=O)c1cccc(C(=O)OCCCCCCC)c1
<b>Mol. weight [g/mol]:</b>	346.46

## Physical Properties

Property code	Value	Unit	Source
gf	-158.90	kJ/mol	Joback Method
hf	-624.09	kJ/mol	Joback Method
hfus	49.57	kJ/mol	Joback Method
hvap	83.55	kJ/mol	Joback Method
log10ws	-6.41		Crippen Method
logp	5.327		Crippen Method
mcvol	293.570	ml/mol	McGowan Method
pc	1299.53	kPa	Joback Method
rinpol	2548.00		NIST Webbook
tb	868.28	K	Joback Method
tc	1073.05	K	Joback Method
tf	504.61	K	Joback Method
vc	1.131	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	910.28	J/molxK	868.28	Joback Method
cpg	979.03	J/molxK	1038.92	Joback Method
cpg	967.35	J/molxK	1004.80	Joback Method
cpg	954.67	J/molxK	970.67	Joback Method
cpg	940.96	J/molxK	936.54	Joback Method
cpg	926.18	J/molxK	902.41	Joback Method
cpg	989.75	J/molxK	1073.05	Joback Method
dvisc	0.0000416	Paxs	868.28	Joback Method
dvisc	0.0000538	Paxs	807.67	Joback Method

dvisc	0.0000726	Paxs	747.06	Joback Method
dvisc	0.0001033	Paxs	686.44	Joback Method
dvisc	0.0001573	Paxs	625.83	Joback Method
dvisc	0.0002623	Paxs	565.22	Joback Method
dvisc	0.0004944	Paxs	504.61	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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=U356690&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356690&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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