

# Isophthalic acid, di(trans-hex-3-enyl) ester

<b>Inchi:</b>	InChI=1S/C20H26O4/c1-3-5-7-9-14-23-19(21)17-12-11-13-18(16-17)20(22)24-15-10-8-6
<b>InchiKey:</b>	WZABUZCDGHEXSO-KQQUZDAGSA-N
<b>Formula:</b>	C20H26O4
<b>SMILES:</b>	CCC=CCCOC(=O)c1cccc(C(=O)OCCC=CCC)c1
<b>Mol. weight [g/mol]:</b>	330.42

## Physical Properties

Property code	Value	Unit	Source
gf	-87.10	kJ/mol	Joback Method
hf	-486.23	kJ/mol	Joback Method
hfus	47.19	kJ/mol	Joback Method
hvap	81.28	kJ/mol	Joback Method
log10ws	-5.85		Crippen Method
logp	4.713		Crippen Method
mvol	275.180	ml/mol	McGowan Method
pc	1450.14	kPa	Joback Method
rinpol	2414.00		NIST Webbook
tb	849.56	K	Joback Method
tc	1058.23	K	Joback Method
tf	488.26	K	Joback Method
vc	1.056	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	824.64	J/molxK	849.56	Joback Method
cpg	839.86	J/molxK	884.34	Joback Method
cpg	854.07	J/molxK	919.12	Joback Method
cpg	867.31	J/molxK	953.90	Joback Method
cpg	879.63	J/molxK	988.67	Joback Method
cpg	891.09	J/molxK	1023.45	Joback Method
cpg	901.72	J/molxK	1058.23	Joback Method
dvisc	0.0005054	Paxs	488.26	Joback Method
dvisc	0.0002654	Paxs	548.48	Joback Method

dvisc	0.0001583	Paxs	608.69	Joback Method
dvisc	0.0001036	Paxs	668.91	Joback Method
dvisc	0.0000727	Paxs	729.13	Joback Method
dvisc	0.0000539	Paxs	789.34	Joback Method
dvisc	0.0000417	Paxs	849.56	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=U356696&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356696&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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