

# Isophthalic acid, pentyl 3-phenylpropyl ester

<b>Inchi:</b>	InChI=1S/C22H26O4/c1-2-3-7-15-25-21(23)19-13-8-14-20(17-19)22(24)26-16-9-12-18-1
<b>InchiKey:</b>	NPFWUMKNSHJKFM-UHFFFAOYSA-N
<b>Formula:</b>	C22H26O4
<b>SMILES:</b>	CCCCCOC(=O)c1cccc(C(=O)OCCc2ccccc2)c1
<b>Mol. weight [g/mol]:</b>	354.44

## Physical Properties

Property code	Value	Unit	Source
gf	-118.29	kJ/mol	Joback Method
hf	-525.42	kJ/mol	Joback Method
hfus	46.00	kJ/mol	Joback Method
hvap	88.09	kJ/mol	Joback Method
log10ws	-6.08		Crippen Method
logp	4.823		Crippen Method
mvol	288.200	ml/mol	McGowan Method
pc	1489.58	kPa	Joback Method
rinpol	2897.00		NIST Webbook
rinpol	2897.00		NIST Webbook
tb	913.68	K	Joback Method
tc	1135.36	K	Joback Method
tf	547.38	K	Joback Method
vc	1.099	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	897.84	J/molxK	913.68	Joback Method
cpg	912.17	J/molxK	950.63	Joback Method
cpg	925.19	J/molxK	987.57	Joback Method
cpg	936.93	J/molxK	1024.52	Joback Method
cpg	947.44	J/molxK	1061.47	Joback Method
cpg	956.76	J/molxK	1098.41	Joback Method
cpg	964.94	J/molxK	1135.36	Joback Method
dvisc	0.0004215	Paxs	547.38	Joback Method

dvisc	0.0002373	Paxs	608.43	Joback Method
dvisc	0.0001483	Paxs	669.48	Joback Method
dvisc	0.0001003	Paxs	730.53	Joback Method
dvisc	0.0000721	Paxs	791.58	Joback Method
dvisc	0.0000543	Paxs	852.63	Joback Method
dvisc	0.0000424	Paxs	913.68	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=U344389&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U344389&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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