

# Isophthalic acid, hexyl 4-nitrophenyl ester

**Inchi:** InChI=1S/C20H21NO6/c1-2-3-4-5-13-26-19(22)15-7-6-8-16(14-15)20(23)27-18-11-9-17(24)  
**InchiKey:** GJTXPZBOURVWDP-UHFFFAOYSA-N  
**Formula:** C20H21NO6  
**SMILES:** CCCCCCOC(=O)c1cccc(C(=O)Oc2ccc([N+](=O)[O-])cc2)c1  
**Mol. weight [g/mol]:** 371.38

## Physical Properties

Property code	Value	Unit	Source
gf	-109.21	kJ/mol	Joback Method
hf	-506.37	kJ/mol	Joback Method
hfus	51.79	kJ/mol	Joback Method
hvap	100.89	kJ/mol	Joback Method
log10ws	-6.54		Crippen Method
logp	4.551		Crippen Method
mcvol	277.440	ml/mol	McGowan Method
pc	1733.22	kPa	Joback Method
rinpol	3183.00		NIST Webbook
rinpol	3183.00		NIST Webbook
tb	1024.74	K	Joback Method
tc	1269.43	K	Joback Method
tf	680.97	K	Joback Method
vc	1.069	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	875.97	J/mol×K	1024.74	Joback Method
cpg	885.81	J/mol×K	1065.52	Joback Method
cpg	894.23	J/mol×K	1106.30	Joback Method
cpg	901.28	J/mol×K	1147.09	Joback Method
cpg	907.01	J/mol×K	1187.87	Joback Method
cpg	911.45	J/mol×K	1228.65	Joback Method
cpg	914.67	J/mol×K	1269.43	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U344683&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U344683&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>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>hvpap:</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>rinppl:</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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