

# Isophthalic acid, 4-nitrophenyl octyl ester

<b>Inchi:</b>	InChI=1S/C22H25NO6/c1-2-3-4-5-6-7-15-28-21(24)17-9-8-10-18(16-17)22(25)29-20-13-
<b>InchiKey:</b>	JSMXPMXECVKZRF-UHFFFAOYSA-N
<b>Formula:</b>	C22H25NO6
<b>SMILES:</b>	CCCCCCCCOC(=O)c1cccc(C(=O)Oc2ccc([N+](=O)[O-])cc2)c1
<b>Mol. weight [g/mol]:</b>	399.44

## Physical Properties

Property code	Value	Unit	Source
gf	-92.37	kJ/mol	Joback Method
hf	-547.65	kJ/mol	Joback Method
hfus	56.97	kJ/mol	Joback Method
hvap	105.34	kJ/mol	Joback Method
log10ws	-7.38		Crippen Method
logp	5.331		Crippen Method
mvol	305.620	ml/mol	McGowan Method
pc	1486.14	kPa	Joback Method
rinpol	3402.00		NIST Webbook
rinpol	3402.00		NIST Webbook
tb	1070.50	K	Joback Method
tc	1316.39	K	Joback Method
tf	703.51	K	Joback Method
vc	1.181	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	993.01	J/molxK	1070.50	Joback Method
cpg	1002.84	J/molxK	1111.48	Joback Method
cpg	1011.19	J/molxK	1152.46	Joback Method
cpg	1018.12	J/molxK	1193.45	Joback Method
cpg	1023.68	J/molxK	1234.43	Joback Method
cpg	1027.95	J/molxK	1275.41	Joback Method
cpg	1030.98	J/molxK	1316.39	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U344685&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U344685&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>hvp:</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>rinp:</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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