

# 3-Nitrophenol, isoBOC

<b>Inchi:</b>	InChI=1S/C11H13NO5/c1-8(2)7-16-11(13)17-10-5-3-4-9(6-10)12(14)15/h3-6,8H,7H2,1-2
<b>InchiKey:</b>	ZFHCIFQZJIAZEI-UHFFFAOYSA-N
<b>Formula:</b>	C11H13NO5
<b>SMILES:</b>	CC(C)COC(=O)Oc1cccc([N+](=O)[O-])c1
<b>Mol. weight [g/mol]:</b>	239.22

## Physical Properties

Property code	Value	Unit	Source
gf	-161.29	kJ/mol	Joback Method
hf	-438.37	kJ/mol	Joback Method
hfus	29.71	kJ/mol	Joback Method
hvap	70.79	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	2.766		Crippen Method
mvol	172.820	ml/mol	McGowan Method
pc	2744.03	kPa	Joback Method
rinpol	1765.00		NIST Webbook
rinpol	1765.00		NIST Webbook
tb	732.85	K	Joback Method
tc	966.70	K	Joback Method
tf	475.67	K	Joback Method
vc	0.661	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.00	J/mol×K	732.85	Joback Method
cpg	483.69	J/mol×K	771.82	Joback Method
cpg	495.38	J/mol×K	810.80	Joback Method
cpg	506.06	J/mol×K	849.77	Joback Method
cpg	515.76	J/mol×K	888.75	Joback Method
cpg	524.47	J/mol×K	927.72	Joback Method
cpg	532.21	J/mol×K	966.70	Joback Method

# Sources

<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=R235148&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R235148&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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>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>rinpola:</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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