

# 3-Hydroxy-4-nitrobenzoic acid

<b>Other names:</b>	4-Nitro-3-hydroxybenzoic acid Benzoic acid, 3-hydroxy-4-nitro-
<b>Inchi:</b>	InChI=1S/C7H5NO5/c9-6-3-4(7(10)11)1-2-5(6)8(12)13/h1-3,9H,(H,10,11)
<b>InchiKey:</b>	XLDLRRGZWIEEHT-UHFFFAOYSA-N
<b>Formula:</b>	C7H5NO5
<b>SMILES:</b>	O=C(O)c1ccc([N+](=O)[O-])c(O)c1
<b>Mol. weight [g/mol]:</b>	183.12
<b>CAS:</b>	619-14-7

## Physical Properties

Property code	Value	Unit	Source
gf	-273.97	kJ/mol	Joback Method
hf	-415.63	kJ/mol	Joback Method
hfus	30.37	kJ/mol	Joback Method
hvap	87.14	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	0.999		Crippen Method
mvol	116.460	ml/mol	McGowan Method
pc	6318.86	kPa	Joback Method
tb	769.73	K	Joback Method
tc	1010.82	K	Joback Method
tf	573.67	K	Joback Method
vc	0.393	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.18	J/molxK	769.73	Joback Method
cpg	308.59	J/molxK	809.91	Joback Method
cpg	314.62	J/molxK	850.09	Joback Method
cpg	320.35	J/molxK	890.28	Joback Method
cpg	325.89	J/molxK	930.46	Joback Method
cpg	331.30	J/molxK	970.64	Joback Method
cpg	336.69	J/molxK	1010.82	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C619147&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C619147&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>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>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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