

# 4-Hydroxy-3-nitrophenylacetic acid

<b>Other names:</b>	3-Nitro-4-hydroxy phenylacetic acid Benzeneacetic acid, 4-hydroxy-3-nitro-
<b>Inchi:</b>	InChI=1S/C8H7NO5/c10-7-2-1-5(4-8(11)12)3-6(7)9(13)14/h1-3,10H,4H2,(H,11,12)
<b>InchiKey:</b>	QBHBHOSRLDPIHG-UHFFFAOYSA-N
<b>Formula:</b>	C8H7NO5
<b>SMILES:</b>	O=C(O)Cc1ccc(O)c([N+](=O)[O-])c1
<b>Mol. weight [g/mol]:</b>	197.14
<b>CAS:</b>	10463-20-4

## Physical Properties

Property code	Value	Unit	Source
gf	-265.55	kJ/mol	Joback Method
hf	-436.27	kJ/mol	Joback Method
hfus	32.96	kJ/mol	Joback Method
hvap	89.37	kJ/mol	Joback Method
log10ws	-1.57		Crippen Method
logp	0.927		Crippen Method
mvol	130.550	ml/mol	McGowan Method
pc	5454.60	kPa	Joback Method
tb	792.61	K	Joback Method
tc	1029.34	K	Joback Method
tf	584.94	K	Joback Method
vc	0.449	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.02	J/molxK	792.61	Joback Method
cpg	359.28	J/molxK	832.06	Joback Method
cpg	366.15	J/molxK	871.52	Joback Method
cpg	372.71	J/molxK	910.97	Joback Method
cpg	379.05	J/molxK	950.43	Joback Method
cpg	385.25	J/molxK	989.88	Joback Method
cpg	391.41	J/molxK	1029.34	Joback Method

# Sources

<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=C10463204&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C10463204&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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>h vap:</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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