

# Benzoic acid, p-(3-methyl-3-nitrosoureido)-

**Inchi:** InChI=1S/C9H9N3O4/c1-12(11-16)9(15)10-7-4-2-6(3-5-7)8(13)14/h2-5H,1H3,(H,10,15)(H,11,12,13,14)  
**InchiKey:** LUAOYJDDQIIDIN-UHFFFAOYSA-N  
**Formula:** C9H9N3O4  
**SMILES:** CN(N=O)C(=O)Nc1ccc(C(=O)O)cc1  
**Mol. weight [g/mol]:** 223.19  
**CAS:** 90349-65-8

## Physical Properties

Property code	Value	Unit	Source
hf	-428.61	kJ/mol	Joback Method
hvap	86.31	kJ/mol	Joback Method
log10ws	-2.47		Crippen Method
logp	1.530		Crippen Method
mcvol	154.430	ml/mol	McGowan Method
pc	4135.61	kPa	Joback Method
tb	762.91	K	Joback Method
tc	968.57	K	Joback Method

## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C90349658&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## Legend

**hf:** Enthalpy of formation at standard conditions  
**hvap:** Enthalpy of vaporization at standard conditions  
**log10ws:** 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

Latest version available from:

<https://www.chemeo.com/cid/62-727-6/Benzoic-acid-p-3-methyl-3-nitrosoureido.pdf>

Generated by Cheméo on 2024-04-19 17:52:30.094588289 +0000 UTC m=+15838399.015165601.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.