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

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

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

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature