Benzenamine, N-hydroxy-

Other names:	Aniline, N-hydroxy-
	Hydroxylamine, N-phenyl-
	N-Hydroxyaniline
	N-Hydroxybenzenamine
	N-Phenylhydroxylamine
	NCI-C60093
	NSC 223099
	Phenylhydroxyamine
	Phenylhydroxylamine
	«beta»-Phenylhydroxylamine
	Â«betaÂ»-Phenylhydroxylamine
Inchi:	InChI=1S/C6H7NO/c8-7-6-4-2-1-3-5-6/h1-5,7-8H
InchiKey:	CKRZKMFTZCFYGB-UHFFFAOYSA-N
Formula:	C6H7NO
SMILES:	ONc1ccccc1
Mol. weight [g/mol]:	109.13
CAS:	100-65-2

Physical Properties

Property code	Value	Unit	Source
gf	64.62	kJ/mol	Joback Method
hf	-29.40	kJ/mol	Joback Method
hfus	14.52	kJ/mol	Joback Method
hvap	54.34	kJ/mol	Joback Method
log10ws	-0.74		Aqueous Solubility Prediction Method
logp	1.488		Crippen Method
mcvol	87.490	ml/mol	McGowan Method
pc	5422.51	kPa	Joback Method
tb	505.71	K	Joback Method
tc	710.18	K	Joback Method
tf	352.15 ± 2.00	K	NIST Webbook
tf	356.65	K	Aqueous Solubility Prediction Method
vc	0.318	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	181.75	J/mol×K	505.71	Joback Method
cpg	190.63	J/mol×K	539.79	Joback Method
cpg	198.94	J/mol×K	573.87	Joback Method
cpg	206.73	J/mol×K	607.94	Joback Method
cpg	214.00	J/mol×K	642.02	Joback Method
cpg	220.78	J/mol×K	676.10	Joback Method
cpg	227.11	J/mol×K	710.18	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C100652&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion 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
tf: Normal melting (fusion) point
vc: Critical Volume