1H-Benzotriazole

Other names:	1,2,3-1H-Benzotriazole
	1,2,3-Benzotriazole
	1,2,3-Benztriazole
	1,2,3-Triaza-1H-indene
	1,2,3-Triazaindene
	1,2-Aminoazophenylene
	1H-1,2,3-Benzotriazole
	2,3-Diazaindole
	Azimidobenzene
	Aziminobenzene
	Benzene azimide
	Benzisotriazole
	Benzotriazole
	Benztriazole
	Cobratec 35G
	Cobratec 99
	Cobratec No. 99
	NCI-C03521
	NSC-3058
	U-6233
Inchi:	InChI=1S/C6H5N3/c1-2-4-6-5(3-1)7-9-8-6/h1-4H,(H,7,8,9)
InchiKey:	QRUDEWIWKLJBPS-UHFFFAOYSA-N
Formula:	C6H5N3
SMILES:	c1ccc2[nH]nnc2c1
Mol. weight [g/mol]:	119.12
CAS:	95-14-7

Physical Properties

Property code	Value	Unit	Source
chs	-3315.00	kJ/mol	NIST Webbook
chs	-3325.60 ± 1.00	kJ/mol	NIST Webbook
chs	-3312.20 ± 0.80	kJ/mol	NIST Webbook
hf	335.50 ± 1.30	kJ/mol	NIST Webbook
hfs	236.50 ± 1.20	kJ/mol	NIST Webbook
hfs	250.00 ± 1.10	kJ/mol	NIST Webbook
hsub	97.90	kJ/mol	NIST Webbook
hsub	98.20 ± 0.70	kJ/mol	NIST Webbook

hsub	99.00 ± 0.50	kJ/mol	NIST Webbook
hsub	99.00 ± 0.50	kJ/mol	NIST Webbook
ie	9.20 ± 0.05	eV	NIST Webbook
log10ws	-0.78		Estimated Solubility Method
log10ws	-0.78		Aqueous Solubility Prediction Method
logp	0.476		Crippen Method
mcvol	86.420	ml/mol	McGowan Method
rinpol	1469.00		NIST Webbook
ripol	2629.00		NIST Webbook
tf	371.48	K	Aqueous Solubility Prediction Method
tt	369.26	K	Solution Thermodynamics of Benzotriazole in Different Pure Solvents

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	178.70	J/mol×K	298.15	NIST Webbook
hfust	7.70	kJ/mol	369.90	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Solution Thermodynamics of Benzotriazole in Different Pure Solvents: https://www.doi.org/10.1021/acs.jced.7b01085

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C95147&Units=SI

Legend

chs: Standard solid enthalpy of combustion

cps: Solid phase heat capacity

hf: Enthalpy of formation at standard conditions

hfs:	Solid phase enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature