1H-Benzimidazole

Other names:	1,3-Diazaindene
	1,3-benzodiazole
	3-azaindole
	Azindole
	BZI
	Benziminazole
	Benzoglyoxaline
	Benzoimidazole
	N,N'-Methenyl-o-phenylenediamine
	NSC 759
	benzimidazole
	o-Benzimidazole
Inchi:	InChI=1S/C7H6N2/c1-2-4-7-6(3-1)8-5-9-7/h1-5H,(H,8,9)
InchiKey:	HYZJCKYKOHLVJF-UHFFFAOYSA-N
Formula:	C7H6N2
SMILES:	c1ccc2[nH]cnc2c1
Mol. weight [g/mol]:	118.14
CAS:	51-17-2

Physical Properties

Property code	Value	Unit	Source
affp	953.80	kJ/mol	NIST Webbook
basg	920.50	kJ/mol	NIST Webbook
chs	-3691.60 ± 1.00	kJ/mol	NIST Webbook
chs	-3697.00	kJ/mol	NIST Webbook
hf	181.70 ± 1.40	kJ/mol	NIST Webbook
hfs	79.50 ± 1.30	kJ/mol	NIST Webbook
hsub	102.20 ± 0.40	kJ/mol	NIST Webbook
hsub	94.30 ± 0.60	kJ/mol	NIST Webbook
hsub	102.20 ± 0.40	kJ/mol	NIST Webbook
hsub	102.20	kJ/mol	NIST Webbook
hsub	98.90 ± 0.40	kJ/mol	NIST Webbook
hsub	107.00	kJ/mol	NIST Webbook
ie	8.00	eV	NIST Webbook
ie	8.45	eV	NIST Webbook
ie	8.44	eV	NIST Webbook
ie	8.00	eV	NIST Webbook

log10ws	-2.26		Crippen Method
logp	1.081		Crippen Method
mcvol	90.530	ml/mol	McGowan Method
ripol	2039.00		NIST Webbook
ripol	2039.00		NIST Webbook
tf	445.51	K	Solubility of Imidazoles, Benzimidazoles, and Phenylimidazoles in Dichloromethane, 1-Chlorobutane, Toluene, and 2-Nitrotoluene
tf	445.51	K	Solubility of Benzimidazoles in Alcohols

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	128.80	J/mol×K	298.15	NIST Webbook
hfust	20.47	kJ/mol	445.50	NIST Webbook
hfust	19.25	kJ/mol	443.20	NIST Webbook
hsubt	90.20 ± 0.60	kJ/mol	363.00	NIST Webbook
hsubt	101.80 ± 0.40	kJ/mol	349.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51172&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of Benzimidazoles in Alcohols:	https://www.doi.org/10.1021/je020228x
Solubility of Imidazoles, Benzimidazoles, and Phenylimidazoles in Dichloromethane, 1-Chlorobutane, Toluene, and 2-Nitrotoluene:	https://www.doi.org/10.1021/je049907t

Legend

affp:	Proton affinity
basg:	Gas basicity
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
hsubt:	Enthalpy of sublimation at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ripol:	Polar retention indices
tf:	Normal melting (fusion) point