2,1,3-Benzothiadiazole

Other names:	2-Thia-1,3-diaza-2H-isoindene
	3,4-Benzo-1,2,5-thiadiazole
	Benzisothiadiazole
	piazthiole
Inchi:	InChI=1S/C6H4N2S/c1-2-4-6-5(3-1)7-9-8-6/h1-4H
InchiKey:	PDQRQJVPEFGVRK-UHFFFAOYSA-N
Formula:	C6H4N2S
SMILES:	c1ccc2nsnc2c1
Mol. weight [g/mol]:	136.17
CAS:	273-13-2

Physical Properties

Property code	Value	Unit	Source
hfus	16.30	kJ/mol	2,1,3-Benzothiadiazole: study of its structure, energetics and aromaticity
hsub	70.70 ± 0.20	kJ/mol	NIST Webbook
ie	9.00	eV	NIST Webbook
ie	8.98	eV	NIST Webbook
ie	9.00	eV	NIST Webbook
log10ws	-2.56		Crippen Method
logp	1.691		Crippen Method
mcvol	92.790	ml/mol	McGowan Method
tb	479.20	K	NIST Webbook
tb	479.00	K	NIST Webbook
tf	317.00	K	NIST Webbook

Sources

2,1,3-Benzothiadiazole: study of its structure, energetics and aromaticity:	https://www.doi.org/10.1016/j.jct.2012.02.005
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C273132&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hfus:	Enthalpy of fusion at standard conditions
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point