2-Mercapto-1,3-benzoxazole

Other names:	2(3H)-Benzoxazolethione
	2-Benzoxazolinethione
	2-benzoxazolethiol
	2-mercaptobenzoxazole
	Benzoxazole, 2-mercapto-
	Benzoxazolinethione
	benzoxazole-2-thiol
Inchi:	InChI=1S/C7H5NOS/c10-7-8-5-3-1-2-4-6(5)9-7/h1-4H,(H,8,10)
InchiKey:	FLFWJIBUZQARMD-UHFFFAOYSA-N
Formula:	C7H5NOS
SMILES:	S=c1[nH]c2ccccc2o1
Mol. weight [g/mol]:	151.19
CAS:	2382-96-9

Physical Properties

Property code	Value	Unit	Source
hfus	22.56	kJ/mol	Combustion energies and formation enthalpies of 2-SH-benzazoles
ie	8.14	eV	NIST Webbook
log10ws	-7.08		Crippen Method
logp	2.008		Crippen Method
mcvol	102.770	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	22.60 ± 0.90	kJ/mol	468.30	NIST Webbook
hfust	25.00	kJ/mol	470.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2382969&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Combustion energies and formation enthalpies of 2-SH-benzazoles:	https://www.doi.org/10.1016/j.jct.2008.02.018
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion 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