

# 2-Benzimidazolethiol

**Other names:** 1,3-Dihydro-2H-benzimidazole-2-thione  
1,3-Dihydro-benzoimidazole-2-thione  
1H-Benzimidazol-2-yl hydrosulfide  
1H-Benzimidazole-2-thiol  
1H-Benzo[d]imidazole-2-thiol  
2,3-Dihydro-1H-benzimidazole-2-thiol  
2-Benzimidazolethione  
2-Benzimidazolinethione  
2-Benzimidazolinthion  
2-Mercaptobenzoimidazole  
2-Merkaptobenzimidazol  
2-Thiobenzimidazole  
2-Thiol benzimidazole  
2-mercaptobenzimidazole  
2H-Benzimidazole-2-thione, 1,3-dihydro-  
3030-80-6  
ASM MB  
Anitiegene MB  
Antiegene mb  
Antigen MB  
Antigene MB  
Antioxidant mb  
Aomb  
Mercaptobenzimidazole  
Mercaptobenzoimidazole  
Merkaptobenzimidazol  
NCI-C56268  
NCI-C60980  
NSC 186246  
NSC 21414  
Nocrac MB  
Permanax 21  
USAF EK-6540  
USAF XF-21  
Vulkanox MB  
Vulkanox MBI  
benzimidazol-2-thione  
benzimidazole-2-thiol  
o-Phenyleneithiourea

**Inchi:** InChI=1S/C7H6N2S/c10-7-8-5-3-1-2-4-6(5)9-7/h1-4H,(H2,8,9,10)

**InchiKey:** YHMYGUUIMTVXNW-UHFFFAOYSA-N  
**Formula:** C7H6N2S  
**SMILES:** Sc1nc2ccccc2[nH]1  
**Mol. weight [g/mol]:** 150.20  
**CAS:** 583-39-1

## Physical Properties

Property code	Value	Unit	Source
hfus	24.11	kJ/mol	Combustion energies and formation enthalpies of 2-SH-benzazoles
log10ws	-2.77		Crippen Method
logp	1.370		Crippen Method
mcvol	106.880	ml/mol	McGowan Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	24.11	kJ/mol	589.40	NIST Webbook

## Sources

Solubility Determination and Thermodynamic Modeling of 2-Mercapto-1H-benzimidazole in 12 Solvents from T = 278.15 K to T = 318.15 K.

<https://www.doi.org/10.1021/acs.jced.9b00190>

Crippen Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C583391&Units=SI>

Combustion energies and formation enthalpies of 2-SH-benzazoles:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

<https://www.doi.org/10.1016/j.jct.2008.02.018>

## Legend

hfus: Enthalpy of fusion at standard conditions

**hfust:** Enthalpy of fusion at a given temperature  
**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume

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