

## Product Information

### 2-Iminothiolane hydrochloride

Product Number **I 6256**  
Storage Temperature 2-8 °C

#### Product Description

Molecular Formula: C<sub>4</sub>H<sub>7</sub>NS • HCl  
Molecular Weight: 137.6  
CAS Number: 4781-83-3  
Melting Point: 192-193 °C<sup>1</sup>  
 $\lambda_{\text{max}}$ : 248 nm<sup>1</sup>  
Extinction coefficient: E<sup>mM</sup> = 8.84 (0.1 M HCl)<sup>1</sup>  
Synonyms: dihydro-2(3H)-thiophenimine hydrochloride, 2-thiolanimine hydrochloride, Traut's reagent

2-Iminothiolane is a thiolating reagent that is used in the preparation of disulfide and thioether linked conjugates, such as for protein crosslinking.<sup>1,2,3</sup> It has a preference for primary amino groups and reacts at pH 7-10 to give amidine compounds which contain free sulhydryl groups. The amidine linkage preserves the original primary amine positive charge. A mechanistic study of the reaction of 2-iminothiolane with amino groups in peptides and proteins has been published.<sup>4</sup>

Other biological crosslinks which have been investigated using 2-iminothiolane include RNA-protein contact sites.<sup>5,6</sup> 2-Iminothiolane has been utilized to prepare glycoprotein-antibody conjugates, streptavidin-antibody conjugates, and avidin-protein nanoparticle conjugates.<sup>7,8,9</sup>

#### Precautions and Disclaimer

For Laboratory Use Only. Not for drug, household or other uses.

#### Preparation Instructions

This product is soluble in water (100 mg/ml), with heat as needed, yielding a clear to slightly hazy, colorless to faint yellow solution.

#### References

1. Jue, R., et al., Addition of sulfhydryl groups to *Escherichia coli* ribosomes by protein modification with 2-iminothiolane (methyl 4-mercaptobutyrimidate). *Biochemistry*, **17(25)**, 5399-5406 (1978).
2. Schramm, H. J., and Dulffer, T., The use of 2-iminothiolane as a protein crosslinking reagent. *Hoppe Seylers Z. Physiol. Chem.*, **358(1)**, 137-139 (1977).
3. Sinz, A., and Wang, K., Mapping protein interfaces with a fluorogenic cross-linker and mass spectrometry: application to nebulin-calmodulin complexes. *Biochemistry*, **40(26)**, 7903-7913 (2001).
4. Singh, R., et al., Formation of N-substituted 2-iminothiolanes when amino groups in proteins and peptides are modified by 2-iminothiolane. *Anal. Biochem.*, **236(1)**, 114-125 (1996).
5. Urlaub, H., et al., Protein-rRNA binding features and their structural and functional implications in ribosomes as determined by cross-linking studies. *EMBO J.*, **14(18)**, 4578-4588 (1995).
6. Thiede, B., et al., Identification and sequence analysis of RNA-protein contact sites by N-terminal sequencing and MALDI-MS. *Methods Mol. Biol.*, **118**, 63-72 (1999).
7. Fu, Q., and Gowda, D. C., Carbohydrate-directed conjugation of cobra venom factor to antibody by selective derivatization of the terminal galactose residues. *Bioconjug. Chem.*, **12(2)**, 271-279 (2001).
8. Foulon, C. F., et al., Preparation and characterization of anti-tenascin monoclonal antibody-streptavidin conjugates for pretargeting applications. *Bioconjug. Chem.*, **10(5)**, 867-876 (1999).
9. Langer, K., et al., Preparation of avidin-labeled protein nanoparticles as carriers for biotinylated peptide nucleic acid. *Eur. J. Pharm. Biopharm.*, **49(3)**, 303-307 (2000).

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