

Product Data Sheet

Product Name: HOAt
Cat. No.: GA10098

Chemical Properties

Cas. No. 39968-33-7

Chemical Name 3-hydroxytriazolo[4,5-b]pyridine

SMILES C1=CC2=C(N=C1)N(N=N2)O

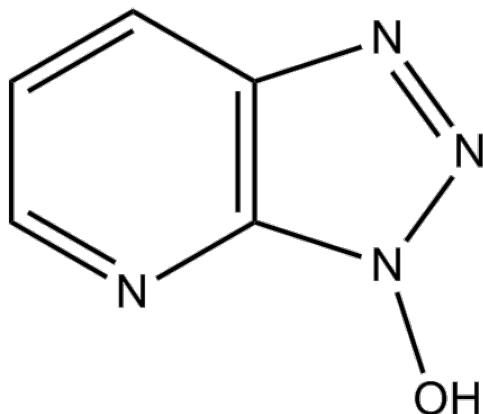
Formula C5H4N4O M.Wt 136.11

Solubility $\geq 6.8\text{mg/mL}$ in DMSO, $\geq 9.29\text{ mg/mL}$ in EtOH with ultrasonic, $\geq 3.62\text{ mg/mL}$ in Water with ultrasonic
Storage Desiccate at -20°C

General tips For obtaining a higher solubility, please warm the tube at 37°C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Shipping Condition Evaluation sample solution: ship with blue ice. All other available size: ship with RT, or blue ice upon request.

Structure



Background

HOAt is a coupling reagent that promotes peptide bond formation between carboxylic acids and amines by first reacting with the acid to generate an activated intermediate, which then reacts with the amine to form the amide^[1]. The nitrogen at the 7-position in HOAt provides a classic neighboring

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group effect that can both increase the reactivity and reduce racemization^[2]. In combination with 1-ethyl-3-(3-(dimethylamino)propyl)carbodiimide (EDC) and *N,N*-diisopropylethylamine (DIPEA), HOAt can be employed to promote the amide-bond-forming step between amino-modified DNA and carboxylic acids during the construction of DNA-encoded combinatorial libraries^[3]. HOAt functions as a non-mutagenic pharmaceutical reagent, a common drug impurity and a metal-binding pharmacophore, while also exhibiting pronounced corrosion-inhibition activity toward mild steel^[4-5]. HOAt can be used with HOBt in a relay fashion to catalyze the route from α -reducible aldehydes and amines to α -reduced amides^[6].

References:

- [1] Nicolette J, Neft RE, Vanosdol J, Murray J. Peptide bond-forming reagents HOAt and HATU are not mutagenic in the bacterial reverse mutation test. *Environ Mol Mutagen*. 2016 Apr;57(3):236-40. doi: 10.1002/em.21997.
- [2] Subirós-Funosas R, Prohens R, Barbas R, El-Faham A, Albericio F. Oxyma: an efficient additive for peptide synthesis to replace the benzotriazole-based HOBt and HOAt with a lower risk of explosion. *Chemistry*. 2009 Sep 21;15(37):9394-403.
- [3] Li Y, Gabriele E, Samain F, et al. Optimized Reaction Conditions for Amide Bond Formation in DNA-Encoded Combinatorial Libraries. *ACS Comb Sci*. 2016;18(8):438-443.
- [4] Liu X, Yan W, Yang G, et al. 1-hydroxy-7-azabenzotriazole-cinnamic esters as anti- *Toxoplasma gondii* agents. *Nat Prod Res*. Published online May 8, 2025.
- [5] Gao L, Peng S, Gong Z, Chen J. A combination of experiment and theoretical methods to study the novel and low-cost corrosion inhibitor 1-hydroxy-7-azabenzotriazole for mild steel in 1 M sulfuric acid. *RSC Adv*. 2018;8(67):38506-38516.
- [6] Vora HU, Rovis T. Nucleophilic carbene and HOAt relay catalysis in an amide bond coupling: an orthogonal peptide bond forming reaction. *J Am Chem Soc*. 2007 Nov 14;129(45):13796-7. doi: 10.1021/ja0764052.

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