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ProductInformation

Isocytosine

Product Number **I 2127**
Store at Room Temperature

Product Description

Molecular Formula: $C_4H_5N_3O$
Molecular Weight: 111.1
CAS Number: 108-53-2
Melting Point: 275 °C
λ_{max}: 225 nm, 273 nm (0.1 N NaOH);
215 nm, 257 nm (0.1 N HCl)[1]
Extinction Coefficient: E^{mM} = 7.78 (225 nm),
6.58 (273 nm) (0.1 N NaOH); 9.40 (215 nm),
6.97 (257 nm) (0.1 N HCl)[1]
Synonym: 2-amino-4-hydroxypyrimidine; iso-C

Isocytosine (iso-C) is a structural isomer of the nucleobase cytosine, where the positions of the carbonyl and exocyclic amine groups are interchanged compared to cytosine. A detailed study of the variations in extinction coefficient of iso-C with pH has been reported.[2] The crystal structure of iso-C has been published.[3] An investigation of the magnetic circular dichroism and circular dichroism spectra of iso-C and other nucleosides has been described.[4]

Iso-C has been studied as a potential prebiotic compound formed during the early history of the earth.[5] Iso-C can base pair in a Watson-Crick manner with the corresponding compound isoguanine, and the enzymatic incorporation of iso-C opposite isoguanine in oligonucleotides has been investigated.[6] An NMR study of double-stranded oligonucleotides that contain iso-C has been published.[7]

The synthesis of antiviral compounds that incorporate an iso-C moiety has been reported.[8,9]

Precautions and Disclaimer

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

Preparation Instructions

This product is soluble in acetic acid (50 mg/ml), with heat as needed, yielding a clear, colorless solution.

References

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7. Yang, X. L., et al., Structural studies of a stable parallel-stranded DNA duplex incorporating isoguanine:cytosine and isocytosine:guanine basepairs by nuclear magnetic resonance spectroscopy. Biophys. J., **75(3)**, 1163-1171 (1998).

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9. Beauchamp, L. M., et al., Effect of acyclic pyrimidines related to 9-[(1,3-dihydroxy-2-propoxy)methyl]guanine on herpesviruses. J. Med. Chem., **31(1)**, 144-149 (1988).

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