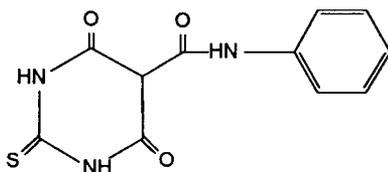


MERBARONE

NSC - 336628



Chemical Name:

Hexahydro-4,6-dioxo-*N*-phenyl-2-thioxo-5-pyridinecarboxamide

Other Names:

5-Carboxyanilino-2-thiobarbituric acid

CAS Registry Number: 97534-21-9

Molecular Formula: C₁₁H₉N₃O₃S

M.W.: 263.3

Approximate Solubility:

(mg/mL)

H ₂ O	< 0.1
C ₂ H ₅ OH	< 0.1
0.1N HCl	< 0.1
DMSO	80
0.1N NaOH	5
CHCl ₃	< 0.1
CH ₃ CN	< 0.1
pH 9 buffer	< 0.1
(CH ₃) ₂ CO	< 0.1

TFA < 0.1
THF 6

Stability:

Bulk:

As a bulk chemical, Merbarone is found to be stable at 25 and 45 °C for at least 4 weeks (HPLC).

Solution:

As a 1 mg/mL pH 9 buffered solution at room temperature (25 ± 2 °C), Merbarone appeared stable for at least 24 hours (HPLC).

Ultraviolet Absorption:

(0.1 N NaOH)

λ_{\max}	ϵ
306 ± 2 nm	29,600 - 30,300
243 ± 2 nm	17,000 - 17,500

High Performance Liquid Chromatography:

Column: Hamilton PRP-1, 250 x 4.1 mm i.d.

Mobile Phase: 14% CH₃CN in 0.1 M Na₂HPO₄ (pH adjusted to 10.2 with NaOH)

Flow Rate: 1.5 mL/min

Detection: UV at 243 nm

Sample Preparation: Approximately 1 mg of sample dissolved in 2 mL of mobile phase plus one drop of 5N NaOH

Retention Volume: 7.3 mL (NSC-336628)