

Product Name: TC-E 5008

Catalog No.: 5244

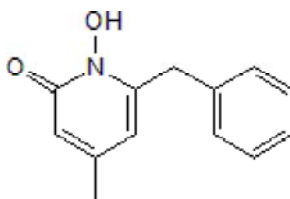
Batch No.: 1

CAS Number: 50405-58-8

IUPAC Name: 1-Hydroxy-4-methyl-6-(phenylmethyl)-2-(1H)pyridinone

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₃H₁₃NO₂
Batch Molecular Weight: 215.25
Physical Appearance: Pale yellow solid
Solubility: DMSO to 100 mM
 ethanol to 100 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.35 (Dichloromethane:Methanol [95:5])
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

| | Carbon | Hydrogen | Nitrogen |
|-------------|--------|----------|----------|
| Theoretical | 72.54 | 6.09 | 6.51 |
| Found | 72.64 | 6.12 | 6.61 |

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Catalog No.: 5244

Batch No.: 1

CAS Number: 50405-58-8

IUPAC Name: 1-Hydroxy-4-methyl-6-(phenylmethyl)-2-(1H)pyridinone

Description:

Selective mutant isocitrate dehydrogenase 1 (mIDH1) inhibitor ($K_i = 120\text{-}190$ nM). Displays >60-fold selectivity for mIDH1 (found in ~75% of gliomas) over wild type IDH1. Also inhibits D-2-hydroxyglutaric acid in cells expressing mIDH1 ($EC_{50} = 2.4$ μM). Does not display cytotoxicity towards non-cancerous human cells. Phenotypically lethal.

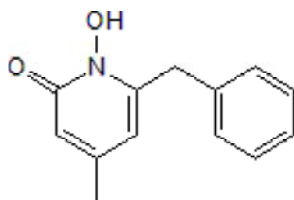
Physical and Chemical Properties:

Batch Molecular Formula: $C_{13}H_{13}NO_2$

Batch Molecular Weight: 215.25

Physical Appearance: Pale yellow solid

Batch Molecular Structure:



References:

Zheng *et al* (2013) Crystallographic investigation and selective inhibition of mutant isocitrate dehydrogenase. ACS Med.Chem.Lett. **4** 542. PMID: 23795241.

Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 100 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

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