

**Product Name:** SR 13800

**Catalog No.:** 5431

**Batch No.:** 1

CAS Number: 227321-12-2

IUPAC Name: 2,6-Dihydro-7-[(3-hydroxypropyl)thio]-2-methyl-4-(2-methylpropyl)-6-(1-naphthalenylmethyl)-1*H*-pyrrolo[3,4-*d*]pyridazin-1one

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>25</sub>H<sub>29</sub>N<sub>3</sub>O<sub>2</sub>S·¼H<sub>2</sub>O

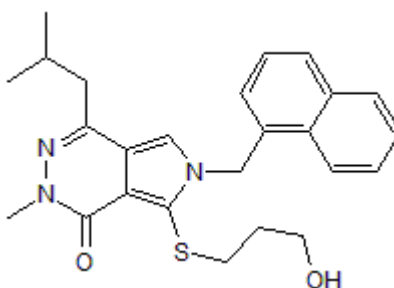
**Batch Molecular Weight:** 440.08

**Physical Appearance:** White solid

**Solubility:** DMSO to 100 mM  
ethanol to 20 mM

**Storage:** Store at +4°C

**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.4 (Ethyl acetate:Petroleum ether [2:3])

**HPLC:** Shows 99.8% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	68.23	6.76	9.55
Found	68.39	6.68	9.55

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**Description:**

Potent MCT1 inhibitor (IC<sub>50</sub> = 0.5 nM); blocks proliferation of Raji lymphoma cells in vitro. Also inhibits lactate uptake in breast cancer cells in vitro.

**Physical and Chemical Properties:**

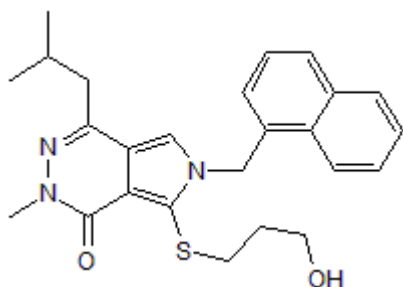
Batch Molecular Formula: C<sub>25</sub>H<sub>29</sub>N<sub>3</sub>O<sub>2</sub>S.¼H<sub>2</sub>O

Batch Molecular Weight: 440.08

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**References:**

**Murray et al** (2005) Monocarboxylate transporter MCT1 is a target for immunosuppression. *Nat.Chem.Biol.* **1** 371. PMID: 16370372.

**Wang et al** (2014) Synthesis and structure-activity relationships of pteridine dione and trione monocarboxylate transporter 1 inhibitors. *J.Med.Chem.* **57** 7317. PMID: 25068893.

**Storage:** Store at +4°C

**CAUTION** - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

**Solubility & Usage Info:**

DMSO to 100 mM

ethanol to 20 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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**bio-techne.com**

info@bio-techne.com

techsupport@bio-techne.com

**North America**

Tel: (800) 343 7475

**China**

info.cn@bio-techne.com

Tel: +86 (21) 52380373

**Europe Middle East Africa**

Tel: +44 (0)1235 529449

**Rest of World**

www.tocris.com/distributors

Tel:+1 612 379 2956