

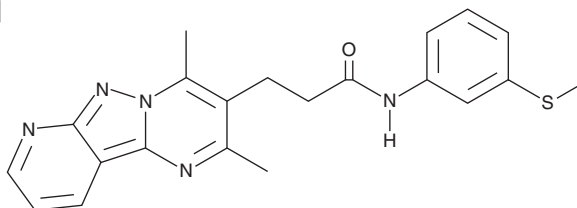
# PRODUCT INFORMATION



## Pantothenate Kinase Inhibitor

Item No. 31002

**CAS Registry No.:** 902614-04-4  
**Formal Name:** 2,4-dimethyl-N-[3-(methylthio)phenyl]-pyrido[2',3':3,4]pyrazolo[1,5-a]pyrimidine-3-propanamide  
**Synonyms:** PANKi, PanK Inhibitor  
**MF:** C<sub>21</sub>H<sub>21</sub>N<sub>5</sub>OS  
**FW:** 391.5  
**Purity:** ≥95%  
**UV/Vis.:** λ<sub>max</sub>: 233, 282 nm  
**Supplied as:** A crystalline solid  
**Storage:** -20°C  
**Stability:** ≥4 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

### Laboratory Procedures

Pantothenate kinase inhibitor is supplied as a crystalline solid. A stock solution may be made by dissolving the pantothenate kinase inhibitor in the solvent of choice, which should be purged with an inert gas. Pantothenate kinase inhibitor is soluble in organic solvents such as DMSO and dimethyl formamide. The solubility of pantothenate kinase inhibitor in these solvents is approximately 1 mg/ml.

Pantothenate kinase inhibitor is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, pantothenate kinase inhibitor should first be dissolved in DMSO and then diluted with the aqueous buffer of choice. Pantothenate kinase inhibitor has a solubility of approximately 0.25 mg/ml in a 1:4 solution of DMSO:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

### Description

Pantothenate kinase inhibitor (PANKi) is a reversible inhibitor of pantothenate kinase (PanK; IC<sub>50</sub>s = 70, 92, and 25 nM for PanK1β, PanK2, and PanK3, respectively), the rate-limiting enzyme in the synthesis of coenzyme A (CoA; Item Nos. 16147 | 21499 | 21722).<sup>1</sup> It binds to the ATP-PanK3 complex with an apparent binding constant of 300 nM and exhibits mixed-type inhibition with respect to ATP and pantothenate. PANKi inhibits CoA biosynthesis in C3A cells (IC<sub>50</sub> = 0.9 μM) with no effect on cell viability when used at concentrations up to 8 μM. PANKi (5 μM) synergizes with BSO to induce ferroptosis in PANC-1 cells and sensitizes the cells to imidazole ketone erastin-induced ferroptosis.<sup>2</sup>

### References

1. Sharma, L.K., Leonardi, R., Lin, W., *et al.* A high-throughput screen reveals new small-molecule activators and inhibitors of pantothenate kinases. *J. Med. Chem.* **58**(3), 1563-1568 (2015).
2. Badgley, M.A., Kremer, D.M., Maurer, H.C., *et al.* Cysteine depletion induces pancreatic tumor ferroptosis in mice. *Science* **368**(6486), 85-89 (2020).

#### WARNING

THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

#### SAFETY DATA

This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the complete Safety Data Sheet, which has been sent via email to your institution.

#### WARRANTY AND LIMITATION OF REMEDY

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#### CAYMAN CHEMICAL

1180 EAST ELLSWORTH RD  
ANN ARBOR, MI 48108 · USA

**PHONE:** [800] 364-9897  
[734] 971-3335

**FAX:** [734] 971-3640

CUSTSERV@CAYMANCHEM.COM  
WWW.CAYMANCHEM.COM