

Product Name: CPI 613

Catalog No.: 5348

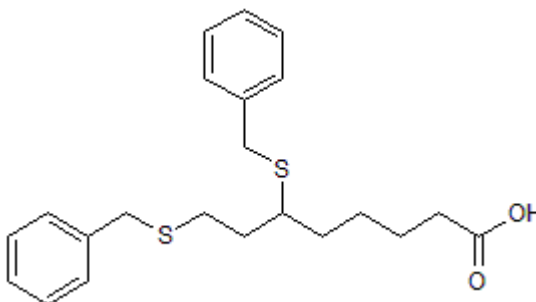
Batch No.: 1

CAS Number: 95809-78-2

IUPAC Name: 6,8-Bis[(phenylmethyl)thio]octanoic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₂H₂₈O₂S₂
Batch Molecular Weight: 388.59
Physical Appearance: White solid
Solubility: DMSO to 100 mM
 ethanol to 100 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.4% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	68	7.26	
Found	68.12	7.37	

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

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CAS Number: 95809-78-2

IUPAC Name: 6,8-Bis[(phenylmethyl)thio]octanoic acid

Description:

Pyruvate dehydrogenase (PDH) and α -ketoglutarate dehydrogenase (KGDH) inhibitor. Disrupts tumor cell mitochondrial metabolism, and increases mitochondrial reactive oxygen species (ROS) production in H460 lung carcinoma cells. Has no effect on KGDH activity in normal bronchial epithelial cells. Induces cell death of multiple tumor cell lines selectively over normal cells in vitro. Inhibits tumor growth of H460 and BxPC-3 tumor cell xenografts in mice.

Physical and Chemical Properties:

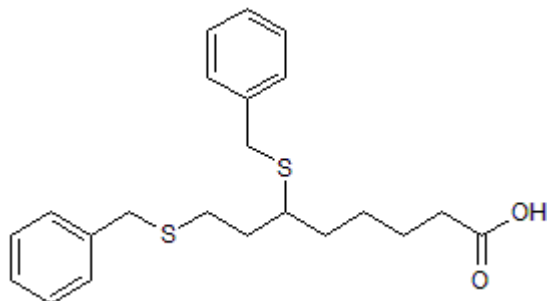
Batch Molecular Formula: $C_{22}H_{28}O_2S_2$

Batch Molecular Weight: 388.59

Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



References:

Zachar et al (2011) Non-redox-active lipoate derivatives disrupt cancer cell mitochondrial metabolism and are potent anticancer agents in vivo. *J.Mol.Med. (Berl.)* **89** 1137. PMID: 21769686.

Stuart et al (2014) A strategically designed small molecule attacks alpha-ketoglutarate dehydrogenase in tumor cells through a redox process. *Cancer Metab.* **2** 4. PMID: 24612826.

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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