

Product data sheet



MedKoo Cat#: 529607 Name: Phenylethyl isothiocyanate CAS: 2257-09-2 Chemical Formula: C ₉ H ₉ NS Exact Mass: 163.0456 Molecular Weight: 163.238		
Product supplied as:		Powder
Purity (by HPLC):		≥ 98%
Shipping conditions		Ambient temperature
Storage conditions:		Powder: -20°C 3 years; 4°C 2 years. In solvent: -80°C 3 months; -20°C 2 weeks.

1. Product description:

Phenylephrine hydrochloride is a phenylephrine and an α 1-adrenoceptor agonist that promotes hypertrophic growth in the ventricular myocytes, and activates several MAPK signaling pathways. It is used as a mydriatic, nasal decongestant, and cardiotonic agent. Phenylephrine hydrochloride is an activator of α 1A-AR, α 1D-AR and α 1B-AR.

2. CoA, QC data, SDS, and handling instruction

SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under “QC And Documents” section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
DMF	30.0	183.78
DMSO	65.0	398.19
Ethanol	30.0	183.78

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	6.13 mL	30.63 mL	61.26 mL
5 mM	1.23 mL	6.13 mL	12.25 mL
10 mM	0.61 mL	3.06 mL	6.13 mL
50 mM	0.12 mL	0.61 mL	1.23 mL

5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator

Please refer the product web page under section of “Calculator”

6. Recommended literature which reported protocols for in vitro and in vivo study

In vitro study

- Zhang M, Li Y, Bi Y, Wang T, Dong Y, Yang Q, Zhang T. 2-Phenylethyl Isothiocyanate Exerts Antifungal Activity against *Alternaria alternata* by Affecting Membrane Integrity and Mycotoxin Production. *Toxins (Basel)*. 2020 Feb 15;12(2):124. doi: 10.3390/toxins12020124. PMID: 32075318; PMCID: PMC7077316.
- Hsu SY, Lee SC, Liu HC, Peng SF, Chueh FS, Lu TJ, Lee HT, Chou YC. Phenethyl Isothiocyanate Suppresses the Proinflammatory Cytokines in Human Glioblastoma Cells through the PI3K/Akt/NF- κ B Signaling Pathway In Vitro. *Oxid Med Cell Longev*. 2022 Mar 25;2022:2108289. doi: 10.1155/2022/2108289. PMID: 35368876; PMCID: PMC8975692.

In vivo study

- Uyumlu AB, Satılmış B, Atıcı B, Taşlıdere A. Phenethyl isothiocyanate protects against cyclophosphamide-induced nephrotoxicity via nuclear factor E2-related factor 2 pathway in rats. *Exp Biol Med (Maywood)*. 2023 Jan;248(2):157-164. doi: 10.1177/15353702221139206. Epub 2023 Jan 4. PMID: 36598044; PMCID: PMC10041055.
- Haloi P, Chawla S, Konkimalla VB. Thermosensitive smart hydrogel of PEITC ameliorates the therapeutic efficacy in rheumatoid arthritis. *Eur J Pharm Sci*. 2023 Feb 1;181:106367. doi: 10.1016/j.ejps.2022.106367. Epub 2022 Dec 23. PMID: 36572358.

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7. Bioactivity

Biological target:

2-Phenylethyl isothiocyanate is a potent antifungal agent.

In vitro activity

The results indicated that PEITC (phenylethyl isothiocyanate) decreased the cell viability and inhibited the protein levels and expressions of IL-1 β , IL-6, and TNF- α genes at the transcriptional level in GBM 8401 cells. PEITC inhibited the binding of NF- κ B on promoter site of DNA in GBM 8401 cells. PEITC also altered the protein expressions of protein kinase B (Akt), extracellular signal-regulated kinase (ERK), and NF- κ B signaling pathways. The inflammatory responses in human glioblastoma cells may be suppressed by PEITC through the phosphoinositide 3-kinase (PI3K)/Akt/NF- κ B signaling pathway.

Reference: Glioblastoma Cells through the PI3K/Akt/NF- κ B Signaling Pathway In Vitro. <https://pubmed.ncbi.nlm.nih.gov/35368876/>

In vivo activity

This study focused to research on the effect of PEITC (phenylethyl isothiocyanate) against renal toxicity caused by CP and its relationship to the Nrf2 signaling mechanism. Thirty female Wistar albino rats were allocated to three groups: control (n = 10), CP (n = 10), and PEITC-pretreated group (150 μ mol/kg b.w. orally; n = 10). Pretreatment with PEITC ameliorated kidney tissue injury. The renal protective effect of the PEITC was supported by the histological analysis of the kidney. PEITC prevented CP-induced nephrotoxicity by decreasing oxidative damage through Nrf2 and SIRT1 activation and NF- κ B inhibition.

Reference: Exp Biol Med (Maywood). 2023 Jan;248(2):157-164. <https://pubmed.ncbi.nlm.nih.gov/36598044/>

Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.