

Product Name: PPT

Catalog No.: 1426

Batch No.: 8

CAS Number: 263717-53-9

IUPAC Name: 4,4',4''-(4-Propyl-[1H]-pyrazole-1,3,5-triyl)trisphenol

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{24}H_{22}N_2O_3 \cdot \frac{1}{4}H_2O$

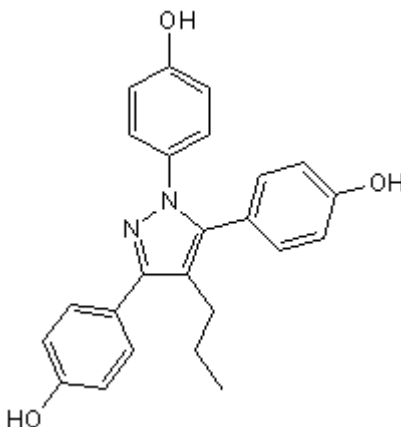
Batch Molecular Weight: 390.95

Physical Appearance: White solid

Solubility: ethanol to 5 mM
DMSO to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: $R_f = 0.55$ (Ethyl acetate:Petroleum ether [3:7])

HPLC: Shows 99.7% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	73.73	5.8	7.17
Found	73.89	5.62	7.2

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

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Description:

Potent, subtype-selective estrogen receptor agonist (EC₅₀ ~ 200 pM); displays 410-fold selectivity for ER α over ER β . Prevents ovariectomy-induced weight gain and loss of bone mineral density, and induces gene expression in the hypothalamus following systemic administration in vivo.

Physical and Chemical Properties:

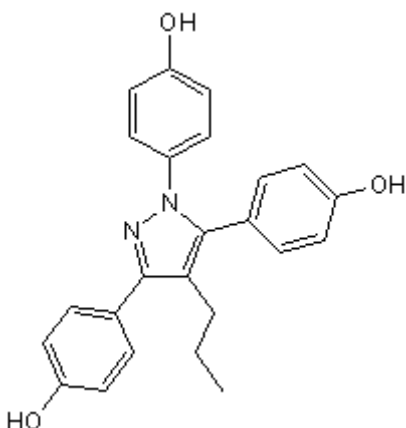
Batch Molecular Formula: C₂₄H₂₂N₂O₃ · ¼H₂O

Batch Molecular Weight: 390.95

Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



References:

Kraichely et al (2000) Conformational changes and coactivator recruitment by novel ligands for estrogen receptor- α and estrogen receptor- β : correlations with biological character and distinct differences among SRC coactivator family members. *Endocrinology* **141** 3534. PMID: 11014206.

Stauffer et al (2000) Pyrazole ligands: structure-affinity/activity relationships and estrogen receptor- α -selective agonists. *J. Med. Chem.* **43** 4934. PMID: 11150164.

Harris et al (2002) Characterization of the biological roles of the estrogen receptors, ER α and ER β , in estrogen target tissues in vivo through the use of an ER α -selective ligand. *Endocrinology* **143** 4172. PMID: 12399409.

Storage: Store at +4°C

Solubility & Usage Info:

ethanol to 5 mM

DMSO to 100 mM

CAUTION - This product is hygroscopic and we recommend that it is desiccated upon arrival. Solutions should be made up as soon as the vial is opened.

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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