

Product Name: MRS 2578

Catalog No.: 2146

Batch No.: 7

CAS Number: 711019-86-2

IUPAC Name: *N,N'*-1,4-Butanediylbis[*N'*-(3-isothiocyanatophenyl)thiourea

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₀H₂₀N₆S₄·C₂H₆SO.

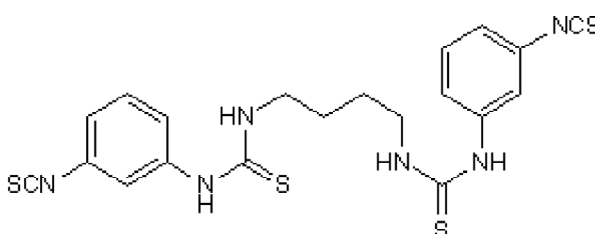
Batch Molecular Weight: 550.79

Physical Appearance: Off-white solid

Solubility: DMSO to 50 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 95.3% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	47.97	4.76	15.26
Found	47.53	4.81	14.89

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CAS Number: 711019-86-2

IUPAC Name: *N,N'*-1,4-Butanediyldis[*N*-(3-isothiocyanatophenyl)thiourea

Description:

MRS 2578 is a selective antagonist of P2Y₆ nucleotide receptors; IC₅₀ values are 37 and 98 nM at human and rat P2Y₆ receptors respectively. Displays no activity at P2Y₁, P2Y₂, P2Y₄ and P2Y₁₁ receptors (IC₅₀ > 10 μM). Inhibits agonist-induced cardiomyocyte contraction and UDP-induced phagocytosis.

Physical and Chemical Properties:

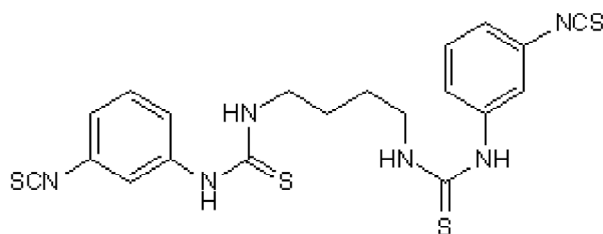
Batch Molecular Formula: C₂₀H₂₀N₆S₄.C₂H₆SO.

Batch Molecular Weight: 550.79

Physical Appearance: Off-white solid

Minimum Purity: ≥95%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 50 mM

CAUTION: Stock solutions of this compound should be prepared in DMSO and used immediately. Analysis shows that when dissolved in aqueous media this compound undergoes rapid hydrolysis to form inactive products.

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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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.

References:

Koizumi *et al* (2007) UDP acting at P2Y₆ receptors is a mediator of microglial phagocytosis. *Nature* **446** 1091. PMID: 17410128.

Kukulski *et al* (2007) Extracellular nucleotides mediate LPS-induced neutrophil migration in vitro and in vivo. *J.Leukoc.Biol.* **81** 1269. PMID: 17322022.

Mamedova *et al* (2004) Diisothiocyanate derivatives as potent, insurmountable antagonists of P2Y₆ nucleotide receptors. *Biochem.Pharmacol.* **67** 1763. PMID: 15081875.

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