

Product Name: Bay 11-7085

Catalog No.: 1743

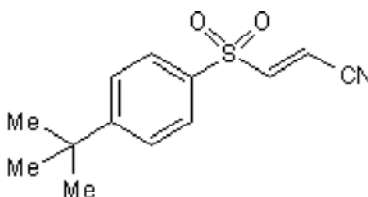
Batch No.: 2

CAS Number: 196309-76-9

IUPAC Name: (2E)-3-[[4-(1,1-Dimethylethyl)phenyl]sulfonyl]-2-propenenitrile

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₃H₁₅NO₂S
Batch Molecular Weight: 249.33
Physical Appearance: White crystalline solid
Solubility: ethanol to 100 mM
DMSO to 100 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.35 (Ethyl acetate:Petroleum ether [1:4])
Melting Point: Between 88 - 90°C
HPLC: Shows 99.3% purity
¹H NMR: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	62.63	6.06	5.62
Found	62.51	6.16	5.52

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

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Description:

Irreversible inhibitor of TNF- α -stimulated I κ B α phosphorylation (IC₅₀ ~ 10 μ M); leads to decreased NF- κ B and subsequent decreased expression of adhesion molecules. Also reversibly activates MAP kinases and stimulates apoptosis. Anti-inflammatory *in vivo*.

Physical and Chemical Properties:

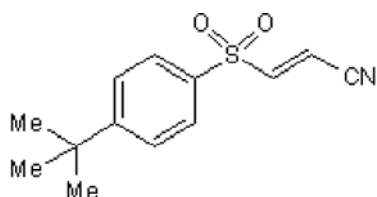
Batch Molecular Formula: C₁₃H₁₅NO₂S

Batch Molecular Weight: 249.33

Physical Appearance: White crystalline solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

ethanol to 100 mM

DMSO 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.

References:

Scaife *et al* (2002) Nuclear factor κ B inhibitors induce adhesion-dependent colon cancer apoptosis: implications for metastasis. *Cancer Res.* **62** 6870. PMID: 12460901.

Hu *et al* (2001) An I κ B α inhibitor causes leukemia cell death through a p38 MAP kinase-dependent, NF- κ B-independent mechanism. *Cancer Res.* **61** 6290. PMID: 11507084.

Pierce *et al* (1997) Novel inhibitors of cytokine-induced I κ B α phosphorylation and endothelial cell adhesion molecule expression show anti-inflammatory effects *in vivo*. *J.Biol.Chem.* **272** 21096. PMID: 9261113.

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