

Unstructured Text

A suspension of 2-cyano-2-(3,4-dichloro-5-oxo-2,5-dihydrofuran-2-yl)acetamide (0.48 g), 2-(aminomethyl)-N-cyclopropyl-4-fluorobenzenesulfonamide obtained in Step 2 (0.60 g) and potassium carbonate (0.85 g) in ethanol (20 ml) was stirred overnight at 70° C. The reaction solution was filtered through celite, and concentrated under reduced pressure.

The residue was purified by basic silica gel column chromatography (ethyl acetate:hexane=7:3-1:0). The obtained residue was dissolved in methanol, 4N hydrogen chloride-ethyl acetate solution (1 ml) was added, and the mixture was crystallized from methanol-ethyl acetate. The precipitated crystals were collected by filtration, and recrystallized from methanol-ethyl acetate to give the title compound (0.06 g).



Structured ord.Reaction Record

Example Compound message

```
{"identifiers": [{"type": "NAME",  
  "value": "ethanol"}],  
"amount": {  
  "volume": { "value": 20.0,  
    "units": "MILLILITER"}},  
"reaction_role": "SOLVENT"}
```

ReactionConditions message

```
{"temperature": {  
  "setpoint": {"value": 70.0,  
    "units": "CELSIUS"}},  
"stirring": {  
  "type": "CUSTOM",  
  "details": "was stirred overnight at 70° C"}}
```

Example ReactionWorkup message

```
{"type": "DISSOLUTION",  
"input": {  
  "components": [{  
    "identifiers": [{"type": "NAME", "value": "methanol"}],  
    "reaction_role": "WORKUP"}]}
```

ReactionOutcome message

```
{"reaction_time": {"value": 8.0, "precision": 8.0, "units": "HOUR"},  
"products": [{"identifiers": [{"type": "NAME",  
  "value": "title compound"}],  
  "measurements": [{  
    "type": "AMOUNT",  
    "amount": {"mass": {"value": 0.06,  
      "units": "GRAM"}}}],  
  "reaction_role": "PRODUCT"}]}
```