



Formula: C<sub>11</sub>H<sub>8</sub>N<sub>2</sub>O

MW: 184.2

CAS: 2826-26-8

MDL NUMBER: MFCD00019787

IUPAC: [(4-methoxyphenyl)methylene]methane-1,1-dicarbonitrile

Smiles: C(/C#N)(C#N)=C/c1ccc(cc1)OC

99%, MW=184.2 [2826-26-8] Storage: RT

ACCEPTORS: 1

DONORS: 0

ROTATION BONDS: 0

N+O: 3

Chiral Centers: 0

LogP: 1.59

LogS: -3.29

LIPINSKI: 4

Synonyms: AKOS USSH-4110227;ALPHA-CYANO-(4-METHOXY)CINNAMONITRILE;AG 9;(4-METHOXYBENZYLIDENE)MALONITRILE;(4-METHOXYBENZYLIDENE)MALONONITRILE;((4-METHOXYPHENYL)METHYLENE)METHANE-1,1-DICARBONITRILE;2-[(4-METHOXYPHENYL)METHYLENE]MALONONITRILE;2-(4-METHOXYBENZYLIDENE)-MALONONITRILE

CAS:2826-26-8

MF:C11H8N2O

MW:184.19

EINECS:

Product Categories: TYRPHOSTIN A1

Chemical Properties: mp 113-116 C(lit.) storage temp. 2-8C Xn Risk Statements 20/21/22  
Safety Statements 36/37 WGK Germany 3 TYRPHOSTIN A1

Usage And Synthesis:

Chemical Properties: light yellow crystalline needles or crystals TYRPHOSTIN A1

