



>>Entry Name: 3-Ethoxy-2-propenenitrile, 9CI

Synonym(s): β -Ethoxyacrylonitrile

CAS Registry Number: 61310-53-0

EtOCH=CHCN

Molecular Formula: C₅H₇NO

Molecular Weight: 97.116

Accurate Mass: 97.052764

Percentage Composition: C 61.84%; H 7.26%; N 14.42%; O 16.47%

Use/Importance: Inexpensive, comly. available synthetic reagent. Synthon for cytosines

Aldrich: 26369-9

>>Variant: (E)-form

CAS Registry Number: 58243-08-6

Molecular Formula: C₅H₇NO

Molecular Weight: 97.116

Accurate Mass: 97.052764

Percentage Composition: C 61.84%; H 7.26%; N 14.42%; O 16.47%

Physical Description: Liq.

Boiling Point: Bp₁₅ 76-78°

Refractive Index: n_D²⁵ 1.4510

>>Variant: (Z)-form

CAS Registry Number: 60036-64-8

Molecular Formula: C₅H₇NO

Molecular Weight: 97.116

Accurate Mass: 97.052764

Percentage Composition: C 61.84%; H 7.26%; N 14.42%; O 16.47%

Physical Description: Liq.

Boiling Point: Bp₁₅ 85-87°

Refractive Index: n_D²⁵ 1.4530

References:

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McElvain, S.M. *et al.*, *J.A.C.S.*, 1947, **69**, 2657, (*synth, props*)

Scotti, F. *et al.*, *J.O.C.*, 1964, **29**, 1800, (*synth, ir, pmr, uv*)

Ford, G.P. *et al.*, *J.C.S. Perkin 2*, 1975, 1371, (*synth, ir, props*)

Movsum-Zade, E.M. *et al.*, *J. Org. Chem. USSR (Engl. Transl.)*, 1977, **13**, 1694, (*synth, ir*)

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