



>>Entry Name: Tetrahydro-2-furancarboxaldehyde, 9CI

Synonym(s): Tetrahydro-2-furaldehyde, 8CI. 2-Formyltetrahydrofuran. Tetrahydrofurfural



CAS Registry Number: 7681-84-7

Molecular Formula: C₅H₈O₂

Molecular Weight: 100.117

Accurate Mass: 100.05243

Percentage Composition: C 59.98%; H 8.05%; O 31.96%

Hazard & Toxicity: LD₅₀ (mus, ipr) 100 mg/kg

Rare Chemicals Library: S62745-3

>>Variant: (R)-form

CAS Registry Number: 22170-11-2

Molecular Formula: C₅H₈O₂

Molecular Weight: 100.117

Accurate Mass: 100.05243

Percentage Composition: C 59.98%; H 8.05%; O 31.96%

Optical Rotation: [α]_D²⁵ -3.4

>>Variant: (S)-form

CAS Registry Number: 22170-12-3

Molecular Formula: C₅H₈O₂

Molecular Weight: 100.117

Accurate Mass: 100.05243

Percentage Composition: C 59.98%; H 8.05%; O 31.96%

Optical Rotation: [α]_D²⁸ +4.2

>>Variant: (±)-form

Molecular Formula: C₅H₈O₂

Molecular Weight: 100.117

Accurate Mass: 100.05243

Percentage Composition: C 59.98%; H 8.05%; O 31.96%

Physical Description: Mobile oil

Boiling Point: Bp₇₇₉ 142-143°. Bp₂₉ 45-47°

>>Derivative: 2,4-Dinitrophenylhydrazone

Physical Description: Pale yellowish-brown prisms (EtOAc)

Melting Point: Mp 130-131°

>>Derivative: Di-Et acetal

Synonym(s): 2-(Diethoxymethyl)tetrahydrofuran

Molecular Formula: C₉H₁₈O₃

Molecular Weight: 174.239

Accurate Mass: 174.125595

Percentage Composition: C 62.04%; H 10.41%; O 27.55%

Boiling Point: Bp 194.5°

References:

Minné, N. *et al.*, *J.A.C.S.*, 1933, **55**, 299, (*synth*)

Defaye, J., *Bull. Soc. Chim. Fr.*, 1968, 2099, (*synth*)

Mottoh, A. *et al.*, *Chem. Comm.*, 1984, 1028