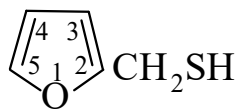




>>Entry Name: 2-Furanmethanethiol, 9CI

ENTRY UNDER REVIEW

Synonym(s): 2-Furfuryl mercaptan. 2-(Mercaptomethyl)furan. FEMA 2493



CAS Registry Number: 98-02-2

Molecular Formula: C₅H₆OS

Molecular Weight: 114.168

Accurate Mass: 114.013935

Percentage Composition: C 52.60%; H 5.30%; O 14.01%; S 28.09%

Source/Synthesis: Formed by thermal treatment of cystine and ribose mixtures. Present in cooked meats, popcorn, wheat bread, roasted coffee and roasted sesame

Use/Importance: Flavour ingredient, along with acetate and propionate. Used in coffee aroma

Physical Description: Liq. with v. disagreeable odour

Boiling Point: Bp 160°. Bp₆₅ 84°

Refractive Index: n_D²⁵ 1.5280

Other Data: Odour becomes coffee-like on dilution. Odour threshol 0.0025ng/L in air and 0.01 µg/kg in H₂O

Hazard & Toxicity: LD₅₀ (mus, ipr) 100 mg/kg. Exp. reprod. effects

Aldrich: F2040-8

Fluka: 48140

Sigma: F0768

>>Derivative: S-Ac

CAS Registry Number: 13678-68-7

Molecular Formula: C₇H₈O₂S

Molecular Weight: 156.205

Accurate Mass: 156.0245

Percentage Composition: C 53.82%; H 5.16%; O 20.49%; S 20.53%

Physical Description: Liq.

Boiling Point: Bp₁₂ 90-92°

Density: d 1.17

Refractive Index: n_D²⁰ 1.5260

>>Derivative: S-Me

Synonym(s): 2-(Methylthiomethyl)furan. FEMA 3160

CAS Registry Number: 1438-91-1

Molecular Formula: C₆H₈OS

Molecular Weight: 128.195

Accurate Mass: 128.029585

Percentage Composition: C 56.22%; H 6.29%; O 12.48%; S 25.01%

Biological Source: Minor constit. of aroma of coffee also present in smoked cured pork and pork liver. Flavour ingredient

Boiling Point: Bp₂₈ 62-63°

Refractive Index: n_D^{22.5} 1.5210

Aldrich: W31600-8

>>Derivative: S-Ph

Synonym(s): 2-(Phenylthiomethyl)furan

CAS Registry Number: 3260-09-1

Molecular Formula: C₁₁H₁₀OS

Molecular Weight: 190.265

Accurate Mass: 190.045235

Percentage Composition: C 69.44%; H 5.30%; O 8.41%; S 16.85%

Physical Description: Oil

Boiling Point: Bp 154°