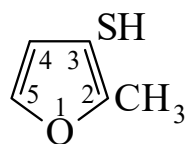




>>Entry Name: 2-Methyl-3-furanthiol, 9CI

Synonym(s): 3-Mercapto-2-methylfuran



CAS Registry Number: 28588-74-1

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%

Use/Importance: Organoleptic compd. with beef broth aroma

Other Data: Well patented. Odour threshold 0.0025 ng/l in air, 0.007µg/l in H₂O

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

Aldrich: W31880-9

>>Derivative: S-Me

Synonym(s): 2-Methyl-3-(methylthio)furan

CAS Registry Number: 63012-97-5

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%

Source/Synthesis: Occurs in coffee and cooked beef aromas. Compd. with intense roasted meat aroma

Use/Importance: Compd. with intense roasted meat aroma

>>Derivative: S-Ph

CAS Registry Number: 105621-16-7

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_{0.9} 100-110°

References:

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U.S. Pat., 1977, 4 020 175; *CA*, **87**, 135020y, (*synth, deriv*)
Moran, E.J. *et al.*, *Drug Chem. Toxicol.*, 1980, **3**, 249, (*tox*)
Tressel, R. *et al.*, *J. Agric. Food Chem.*, 1981, **29**, 1078
MacLeod, G. *et al.*, *Chem. Ind. (London)*, 1986, 175, (*isol, deriv*)
Gasser, U. *et al.*, *Z. Lebensm.-Unters. -Forsch.*, 1988, **186**, 489; 1990, **190**, 3, (*occur*)
McDougal, P.G. *et al.*, *J.O.C.*, 1989, **54**, 91, (*deriv, synth, pmr, ir, ms*)
Kersch, R. *et al.*, *J. Agric. Food Chem.*, 1998, **46**, 1954-1958, (*occur*)