>>**Entry Name: 3,4,5-Trimethylphenol,** 9Cl, 8Cl
Synonym(s): *sym*-Hemimellitenol. 5-Hydroxyhemimellitene

CAS Registry Number: 527-54-8
Extra CAS Registry Numbers(s): 26998-80-1

Molecular Formula: $C_9H_{12}O$
Molecular Weight: 136.193
Accurate Mass: 136.088815
Percentage Composition: C 79.37%; H 8.88%; O 11.75%
Physical Description: Needles with bluish fluor. (hexane)
Melting Point: Mp 108°
Boiling Point: Bp 248-249°
pKa Value: pK_{a1} 10.25 (25°)

Aldrich: 33138-4
Fluka: 92712
Rare Chemicals Library: S42973-2

>>**Derivative:** Ac

CAS Registry Number: 6719-74-0
Molecular Formula: $C_{11}H_{14}O_2$
Molecular Weight: 178.23
Accurate Mass: 178.09938
Percentage Composition: C 74.13%; H 7.92%; O 17.95%
Physical Description: Cryst.
Melting Point: Mp 59-60°

>>**Derivative:** Phenylurethane

Melting Point: Mp 148-149°

>>**Derivative:** Me ether
Synonym(s): 5-Methoxy-1,2,3-trimethylbenzene

CAS Registry Number: 21573-41-1
Molecular Formula: $C_{10}H_{14}O$
Molecular Weight: 150.22
Accurate Mass: 150.104465
Percentage Composition: C 79.96%; H 9.39%; O 10.65%
Boiling Point: Bp_{22} 120°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 283A, *(nmr)*
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Banwell, T. *et al.*, *J.A.C.S.*, 1977, **99**, 3042, *(synth)*
Netzel, D.A.*, Org. Magn. Reson.*, 1978, **11**, 58, *(nmr)*
Baciocchi, E. *et al.*, *J.O.C.*, 1986, **51**, 4544, *(deriv, synth, pmr, ms)*