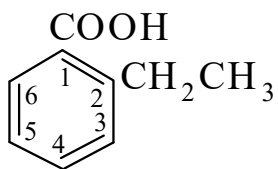




>>Entry Name: 2-Ethylbenzoic acid, 9CI



CAS Registry Number: 612-19-1

Molecular Formula: C₉H₁₀O₂

Molecular Weight: 150.177

Accurate Mass: 150.06808

Percentage Composition: C 71.98%; H 6.71%; O 21.31%

Physical Description: Needles (H₂O)

Melting Point: Mp 68°

Boiling Point: Bp 259°

pKa Value: pK_a 3.79 (25°, H₂O)

Rare Chemicals Library: S62281-8

>>Derivative: Et ester

CAS Registry Number: 56427-44-2

Molecular Formula: C₁₁H₁₄O₂

Molecular Weight: 178.23

Accurate Mass: 178.09938

Percentage Composition: C 74.13%; H 7.92%; O 17.95%

Boiling Point: Bp₇₆₃ 231°

>>Derivative: Chloride

CAS Registry Number: 76118-05-3

Molecular Formula: C₉H₉ClO

Molecular Weight: 168.622

Accurate Mass: 168.034192

Percentage Composition: C 64.11%; H 5.38%; Cl 21.02%; O 9.49%

Boiling Point: Bp_{744.5} 219°

>>Derivative: Amide

CAS Registry Number: 67832-97-7

Molecular Formula: C₉H₁₁NO

Molecular Weight: 149.192

Accurate Mass: 149.084064

Percentage Composition: C 72.46%; H 7.43%; N 9.39%; O 10.72%

Physical Description: Needles (H₂O)

Melting Point: Mp 151-153°

>>Derivative: Nitrile

Synonym(s): 1-Cyano-2-ethylbenzene

CAS Registry Number: 34136-59-9

Molecular Formula: C₉H₉N

Molecular Weight: 131.177

Accurate Mass: 131.073499

Percentage Composition: C 82.41%; H 6.92%; N 10.68%

Boiling Point: Bp 212°

References:

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Stewart, R. *et al.*, *Can. J. Chem.*, 1961, **39**, 2508

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Perez Ossorio, R., *An. R. Soc. Esp. Fis. Quim., Ser. B*, 1966, **62**, 149, (*uv*)