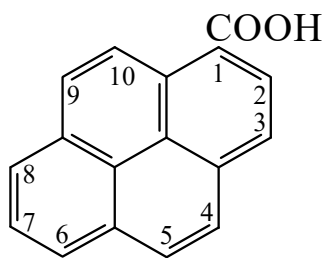




>>Entry Name: 1-Pyrenecarboxylic acid, 9CI

Synonym(s): 3-Pyrenecarboxylic acid (obsol.)



CAS Registry Number: 19694-02-1

Related CAS Registry Numbers(s): 78751-56-1 93638-12-1 113748-27-9

Molecular Formula: C₁₇H₁₀O₂

Molecular Weight: 246.265

Accurate Mass: 246.06808

Percentage Composition: C 82.91%; H 4.09%; O 12.99%

Use/Importance: Fluorescent label for amines

Physical Description: Sl. yellow needles (PhCl or PhNO₂)

Melting Point: Mp 274° (268-269°)

pKa Value: pK_a 3.8 (H₂O)

Other Data: Strong yellow-green fluorescence in conc. sulfuric acid

Aldrich: 39158-1

>>Derivative: Me ester

CAS Registry Number: 6145-35-3

Molecular Formula: C₁₈H₁₂O₂

Molecular Weight: 260.292

Accurate Mass: 260.08373

Percentage Composition: C 83.06%; H 4.65%; O 12.29%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 83-84° (80-81°)

>>Derivative: Et ester

CAS Registry Number: 29556-35-2

Molecular Formula: C₁₉H₁₄O₂

Molecular Weight: 274.318

Accurate Mass: 274.09938

Percentage Composition: C 83.19%; H 5.14%; O 11.66%

Physical Description: Needles (EtOH)

Melting Point: Mp 56° (63°)

>>Derivative: Chloride

Molecular Formula: C₁₇H₉ClO

Molecular Weight: 264.71

Accurate Mass: 264.034192

Percentage Composition: C 77.14%; H 3.43%; Cl 13.39%; O 6.04%

Physical Description: Solid (C₆H₆)

Melting Point: Mp 141°

References:

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Berg, A., *Acta Chem. Scand.*, 1956, **10**, 1362
Neunhoeffter, O. *et al.*, *Annalen*, 1956, **600**, 34, (*synth, acid, Me ester*)
Shozda, R.J. *et al.*, *J.A.C.S.*, 1956, **78**, 1716, (*synth*)
Martin, R.H. *et al.*, *Bull. Soc. Chim. Belg.*, 1965, **74**, 418, (*Me ester, pmr*)
Hansen, P.E. *et al.*, *Org. Magn. Reson.*, 1975, **7**, 23, (*cmr*)
Hansen, P.E. *et al.*, *Acta Chem. Scand., Ser. B*, 1981, **35**, 131, (*ir*)
Milosavljevic, B.H. *et al.*, *J. Phys. Chem.*, 1988, **92**, 2997, (*pKa, props, photophys*)
D'Sousa, L.J. *et al.*, *J.O.C.*, 1996, **61**, 9494-9502, (*synth, Me ester, chloride*)