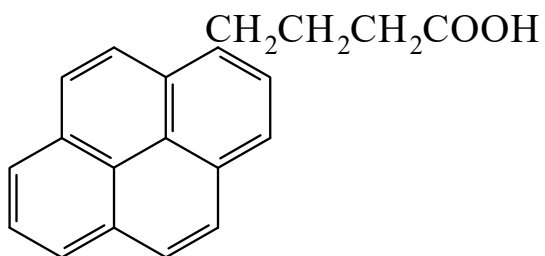




>>Entry Name: 1-Pyrenebutanoic acid, 9Cl, 8Cl



CAS Registry Number: 3443-45-6

Molecular Formula: C₂₀H₁₆O₂

Molecular Weight: 288.345

Accurate Mass: 288.11503

Percentage Composition: C 83.31%; H 5.59%; O 11.10%

Physical Description: Cryst. (AcOH)

Melting Point: Mp 190-190.5°

Aldrich: 25735-4

Fluka: 82655

Sigma: P1407

>>Derivative: Me ester

CAS Registry Number: 70570-29-5

Molecular Formula: C₂₁H₁₈O₂

Molecular Weight: 302.372

Accurate Mass: 302.13068

Percentage Composition: C 83.42%; H 6.00%; O 10.58%

Physical Description: Needles (hexane)

Melting Point: Mp 51.5-52°

>>Derivative: Et ester

CAS Registry Number: 59275-39-7

Molecular Formula: C₂₂H₂₀O₂

Molecular Weight: 316.399

Accurate Mass: 316.14633

Percentage Composition: C 83.52%; H 6.37%; O 10.11%

Physical Description: Prisms (C₆H₆)

Melting Point: Mp 48.5-49°

Boiling Point: Bp 245-247°

References:

Olszak, T.A. *et al.*, *Acta Cryst. C*, 1989, **45**, 803-805, (*cryst struct*)

Werner, F. *et al.*, *Helv. Chim. Acta*, 2000, **83**, 465-478, (*synth, pmr, cmr*)