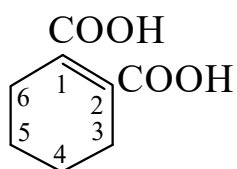




>>Entry Name: 1-Cyclohexene-1,2-dicarboxylic acid, 9CI

Synonym(s): Δ^1 -Tetrahydrophthalic acid



CAS Registry Number: 635-08-5

Molecular Formula: C₈H₁₀O₄

Molecular Weight: 170.165

Accurate Mass: 170.05791

Percentage Composition: C 56.47%; H 5.92%; O 37.61%

Physical Description: Plates (H₂O)

Melting Point: Mp 120°

pKa Value: pK_{a1} 3.75; pK_{a2} 5.08 (20°)

Other Data: Forms anhydride before melting

>>Derivative: Di-Et ester

Molecular Formula: C₁₂H₁₈O₄

Molecular Weight: 226.272

Accurate Mass: 226.12051

Percentage Composition: C 63.70%; H 8.02%; O 28.28%

Boiling Point: Bp₁₄ 160°

>>Derivative: Anhydride

Synonym(s): 4,5,6,7-Tetrahydro-1,3-isobenzofurandione

CAS Registry Number: 2426-02-0

Molecular Formula: C₈H₈O₃

Molecular Weight: 152.149

Accurate Mass: 152.047345

Percentage Composition: C 63.15%; H 5.30%; O 31.55%

Physical Description: Plates (Et₂O)

Melting Point: Mp 74°

Solubility: Sol. Et₂O

Other Data: Undergoes spontaneous polym. with 2-methylimidazole

Aldrich: T1400-1

Fluka: 87461

Sigma: T0267

>>Derivative: Monoamide

Molecular Formula: C₈H₁₁NO₃

Molecular Weight: 169.18

Accurate Mass: 169.073894

Percentage Composition: C 56.80%; H 6.55%; N 8.28%; O 28.37%

Physical Description: Needles (EtOH)

Other Data: Dec. at 170°

>>Derivative: Imide

see 4,5,6,7-Tetrahydro-1*H*-isoindole-1,3(2*H*)-dione, [CZB01-S](#)

References:

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Alder, K. *et al.*, *Ber.*, 1938, **71**, 2206, (*synth*)

Buckles, R.E., *Chem. Rev.*, 1957, **57**, 641, (*rev*)

Park, I.H. *et al.*, *Pollimo*, 1990, **14**, 307; *CA*, **115**, 9503s, (*anhydride, polym*)