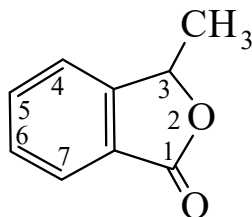




>>Entry Name: 3-Methyl-1(3*H*)-isobenzofuranone, 9CI

Synonym(s): 3-Methylphthalide



CAS Registry Number: 3453-64-3

Molecular Formula: C₉H₈O₂

Molecular Weight: 148.161

Accurate Mass: 148.05243

Percentage Composition: C 72.96%; H 5.44%; O 21.60%

>>Variant: (*R*)-form

CAS Registry Number: 3413-14-7

Molecular Formula: C₉H₈O₂

Molecular Weight: 148.161

Accurate Mass: 148.05243

Percentage Composition: C 72.96%; H 5.44%; O 21.60%

Boiling Point: Bp_{0.9} 101°

Optical Rotation: [α]_D²⁵ +43.3 (c, 0.87 in MeOH)

>>Variant: (*S*)-form

CAS Registry Number: 3205-17-2

Molecular Formula: C₉H₈O₂

Molecular Weight: 148.161

Accurate Mass: 148.05243

Percentage Composition: C 72.96%; H 5.44%; O 21.60%

Physical Description: Needles (pentane/Et₂O); also descr. as an oil

Melting Point: Mp 41.5-42.5°

Optical Rotation: [α]_D²⁵ -50.2 (c, 0.9 in MeOH) (-22.75, claimed 97% op)

>>Variant: (±)-form

Molecular Formula: C₉H₈O₂

Molecular Weight: 148.161

Accurate Mass: 148.05243

Percentage Composition: C 72.96%; H 5.44%; O 21.60%

Melting Point: Mp 8°

Boiling Point: Bp 284.5-285.5° dec.. Bp₂ 115-120°

Other Data: Steam-volatile

References:

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