



>>Entry Name: 3-Piperidinone, 9CI

Synonym(s): β -Piperidone

CAS Registry Number: 50717-82-3

Molecular Formula: C_5H_9NO

Molecular Weight: 99.132

Accurate Mass: 99.068414

Percentage Composition: C 60.58%; H 9.15%; N 14.13%; O 16.14%

>>Derivative: *N*-Ac

CAS Registry Number: 34456-78-5

Molecular Formula: $C_7H_{11}NO_2$

Molecular Weight: 141.169

Accurate Mass: 141.078979

Percentage Composition: C 59.56%; H 7.85%; N 9.92%; O 22.67%

Physical Description: Oil

Boiling Point: $Bp_{0.075}$ 106-108°

>>Derivative: *N*-Me

CAS Registry Number: 5519-50-6

Molecular Formula: $C_6H_{11}NO$

Molecular Weight: 113.159

Accurate Mass: 113.084064

Percentage Composition: C 63.69%; H 9.80%; N 12.38%; O 14.14%

Physical Description: Oil

Boiling Point: Bp_{13} 63-64°

Other Data: Readily oxidized by air

>>Derivative: *N*-Me; hydrochloride

CAS Registry Number: 41511-85-7

Physical Description: Cryst. (Me_2CO)

Melting Point: Mp 110-111°

>>Derivative: *N*-Et

CAS Registry Number: 41361-28-8

Molecular Formula: $C_7H_{13}NO$

Molecular Weight: 127.186

Accurate Mass: 127.099714

Percentage Composition: C 66.11%; H 10.30%; N 11.01%; O 12.58%

Physical Description: Cryst. + $1H_2O$ ($MeOH/Et_2O$) (as hydrochloride)

Melting Point: Mp 178-180° (anhyd.) (hydrochloride)

Other Data: CAS no. refers to hydrochloride

Aldrich: 13048-6

>>Derivative: *N*-Benzyl

CAS Registry Number: 40114-49-6

Molecular Formula: $C_{12}H_{15}NO$

Molecular Weight: 189.257

Accurate Mass: 189.115364

Percentage Composition: C 76.16%; H 7.99%; N 7.40%; O 8.45%

Physical Description: Oil

Boiling Point: $Bp_{1.1}$ 132-133°

Other Data: Free base extremely air-sensitive

>>Derivative: *N*-Benzyl; hydrochloride

CAS Registry Number: 50606-58-1

Melting Point: Mp 168-170°

Boiling Point: $Bp_{0.02}$ 89-91°

Other Data: Forms a covalent hydrate