



>>Entry Name: 4-Octylphenol, 9CI

CAS Registry Number: 1806-26-4

Related CAS Registry Numbers(s): 67367-11-7

Molecular Formula: C<sub>14</sub>H<sub>22</sub>O

Molecular Weight: 206.327

Accurate Mass: 206.167065

Percentage Composition: C 81.50%; H 10.75%; O 7.75%

Physical Description: Needles (petrol)

Melting Point: Mp 44.5°

Boiling Point: Bp<sub>10</sub> 169°. Bp<sub>4</sub> 150°. Bp<sub>1</sub> 134°

Density: d 0.96

Aldrich: 38444-5

Rare Chemicals Library: S55835-4

>>Derivative: Benzoyl

CAS Registry Number: 89202-50-6

Physical Description: Cryst. (EtOH)

Melting Point: Mp 40.5°

>>Derivative: 4-Nitrobenzoyl

CAS Registry Number: 94910-30-2

Physical Description: Cryst. (Me<sub>2</sub>CO)

Melting Point: Mp 81.5°

>>Derivative: 3,5-Dinitrobenzoyl

Melting Point: Mp 91°

>>Derivative: Me ether

Synonym(s): 1-Methoxy-4-octylbenzene

CAS Registry Number: 3307-19-5

Molecular Formula: C<sub>15</sub>H<sub>24</sub>O

Molecular Weight: 220.354

Accurate Mass: 220.182715

Percentage Composition: C 81.76%; H 10.98%; O 7.26%

Melting Point: Mp 17-17.5°

Boiling Point: Bp<sub>1.5</sub> 110-111.5°

Refractive Index: n<sub>D</sub><sup>20</sup> 1.4929

>>Derivative: 3',4'-Didehydro(*E*-)

Synonym(s): 4-(3-Octenyl)phenol. **Gibbilimbol D**

CAS Registry Number: 211806-97-2

Molecular Formula: C<sub>14</sub>H<sub>20</sub>O

Molecular Weight: 204.311

Accurate Mass: 204.151415

Percentage Composition: C 82.30%; H 9.87%; O 7.83%

Biological Source: Constit. of *Piper gibbilimbium*

Biological Use/Importance: Cytotoxic and antibacterial agent

Physical Description: Oil

UV: [neutral] λ<sub>max</sub> 224 (log ε 3.86); 279 (log ε 3.21) (MeOH) [neutral] λ<sub>max</sub> 224 (ε 7720); 279 (ε 1680) (MeOH) (Berdy)

>>Derivative: 4',5'-Didehydro(*E*-)

Synonym(s): 4-(4-Octenyl)phenol. **Gibbilimbol C**

CAS Registry Number: 211806-95-0