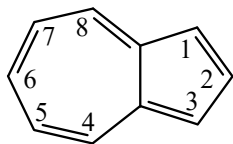




>>Entry Name: Azulene, 9C1

Synonym(s): Bicyclo[5.3.0]deca-1,3,5,7,9-pentaene. Cyclopentacycloheptene



CAS Registry Number: 275-51-4

Molecular Formula: C₁₀H₈

Molecular Weight: 128.173

Accurate Mass: 128.0626

Percentage Composition: C 93.71%; H 6.29%

General Statement: Aromatic hydrocarbon

Biological Source: Occurs in camomile and other essential oils

Use/Importance: Used as a 0.1% soln. in glac. AcOH for photometric detn. of NO₂⁽⁻⁾ ($\lambda_{\max}$ 515 nm, ϵ 52000). Antiinflammatory, antipyretic agent. Used in treatment of anorectal disorders. Alternative to Dihydro-2-thioxo-4,6(1*H*,5*H*)-pyrimidinedione [CTB71-X](#) for detn. of malonaldehyde produced from lipid peroxidation

Physical Description: Greenish-black cryst. or blue needles (hexane)

Melting Point: Mp 100.5-101.5° (99°). Mp 93°

Solubility: Sol. conc. acids, C₆H₆; insol. H₂O

pKa Value: p*K*_a -0.92 (25°, HClO₄ aq.)

Calculated Log P Data: Log P 3.32 (calc)

Other Data: Isomerises to Naphthalene [BNK69-U](#) at 270°. Polymerised chemically or electrochemically to polyazulene, a conducting polymer. Fluoresces in solution. Forms the protonated azulonium cation in conc. acid solution. Permanent dipole moment 0.8 D, with the 7-membered ring +ve

Hazard & Toxicity: Irritant. Low acute oral toxicity. LD₅₀ (rat, ipr) 180 mg/kg

Aldrich: A9720-3

Fluka: 11650

Sigma: A4273

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