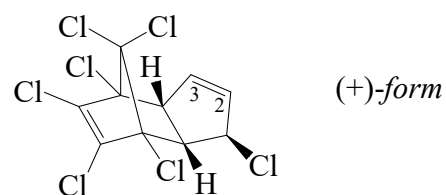




>>Entry Name: Heptachlor, BSI, ISO, JMAF

Synonym(s): 1,4,5,6,7,8,8-Heptachloro-3*a*,4,7,7*a*-tetrahydro-4,7-methano-1*H*-indene, 9Cl. 1-Chlorochlordene. Velsicol 104. Hepta



CAS Registry Number: 76-44-8

Related CAS Registry Numbers(s): 22413-56-5 23720-59-4 68961-31-9

Molecular Formula: C₁₀H₅Cl₇

Molecular Weight: 373.318

Accurate Mass: 369.821089

Percentage Composition: C 32.17%; H 1.35%; Cl 66.48%

Hazard & Toxicity: Toxic effects attributed to the epoxide metabolite. Possible human carcinogen. Hepatotoxic. LD₅₀ (rat, orl) 40 mg/kg. LD₅₀ (rat, skn) 119 mg/kg

Supelco: R42-7140

>>Variant: (+)-form

CAS Registry Number: 74867-73-5

Molecular Formula: C₁₀H₅Cl₇

Molecular Weight: 373.318

Accurate Mass: 369.821089

Percentage Composition: C 32.17%; H 1.35%; Cl 66.48%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 97° (96.1-96.4°)

Optical Rotation: [α]_D²²+209.4 (c, 0.52 in CHCl₃)

>>Derivative: 2β,3β-Epoxyde

Synonym(s): *cis*-Heptachlor epoxide

CAS Registry Number: 145213-11-2

Extra CAS Registry Numbers(s): 1024-57-3

Molecular Formula: C₁₀H₅Cl₇O

Molecular Weight: 389.318

Accurate Mass: 385.816004

Percentage Composition: C 30.85%; H 1.29%; Cl 63.74%; O 4.11%

Metabolism: Metab. of heptachlor

Physical Description: Cryst. (EtOH)

Melting Point: Mp 166°

Optical Rotation: [α]_D−94.1 (c, 0.22 in CHCl₃)

>>Variant: (−)-form

CAS Registry Number: 74867-72-4

Molecular Formula: C₁₀H₅Cl₇

Molecular Weight: 373.318

Accurate Mass: 369.821089

Percentage Composition: C 32.17%; H 1.35%; Cl 66.48%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 97° (96.1-96.4°)

Optical Rotation: [α]_D²²−210.9 (c, 0.54 in CHCl₃)

>>Derivative: 2β,3β-Epoxyde

CAS Registry Number: 66429-34-3

Extra CAS Registry Numbers(s): 1024-57-3

Molecular Formula: C₁₀H₅Cl₇O

Molecular Weight: 389.318

Accurate Mass: 385.816004

Percentage Composition: C 30.85%; H 1.29%; Cl 63.74%; O 4.11%

Melting Point: Mp 166°

Optical Rotation: [α]_D+92.8 (c, 0.21 in CHCl₃)