



>>Entry Name: Pentachlorobenzenethiol, 9Cl

Synonym(s): Pentachlorophenyl mercaptan

CAS Registry Number: 133-49-3

Related CAS Registry Numbers(s): 22441-28-7 22441-29-8

(C<sub>6</sub>Cl<sub>5</sub>)SH

Molecular Formula: C<sub>6</sub>HCl<sub>5</sub>S

Molecular Weight: 282.403

Accurate Mass: 279.824155

Percentage Composition: C 25.52%; H 0.36%; Cl 62.77%; S 11.35%

Metabolism: Metab. of Hexachlorobenzene [FBQ06-P](#) and Pentachloronitrobenzene [FDD48-E](#)

Use/Importance: Vulcanisation accelerator. Peptising agent for natural rubber. Marker for Hexachlorobenzene [FBQ06-P](#) exposure in humans

Physical Description: Cryst. (C<sub>6</sub>H<sub>6</sub>)

Melting Point: Mp 242-244°

>>Derivative: Zn(II) salt

CAS Registry Number: 117-97-5

Use/Importance: Peptising agent for natural rubber processing

Other Data: Mp >300°

>>Derivative: S-Me

Synonym(s): Pentachloro(methylthio)benzene, 9Cl. Methyl pentachlorophenyl sulfide, 8Cl

CAS Registry Number: 1825-19-0

Molecular Formula: C<sub>7</sub>H<sub>3</sub>Cl<sub>5</sub>S

Molecular Weight: 296.43

Accurate Mass: 293.839805

Percentage Composition: C 28.36%; H 1.02%; Cl 59.80%; S 10.82%

Metabolism: Metab. of Pentachloronitrobenzene [FDD48-E](#)

Physical Description: Cryst. (EtOH)

Melting Point: Mp 95-96°

>>Derivative: S-Et

Synonym(s): Pentachloro(ethylthio)benzene, 9Cl. Ethyl pentachlorophenyl sulfide, 8Cl

CAS Registry Number: 77876-27-8

Molecular Formula: C<sub>8</sub>H<sub>5</sub>Cl<sub>5</sub>S

Molecular Weight: 310.457

Accurate Mass: 307.855455

Percentage Composition: C 30.95%; H 1.62%; Cl 57.10%; S 10.33%

Physical Description: Needles (MeOH)

Melting Point: Mp 51-52°

>>Derivative: Disulfide

Synonym(s): Bis(pentachlorophenyl) disulfide

CAS Registry Number: 22441-21-0

Molecular Formula: C<sub>12</sub>Cl<sub>10</sub>S<sub>2</sub>

Molecular Weight: 562.791

Accurate Mass: 557.63266

Percentage Composition: C 25.61%; Cl 62.99%; S 11.40%

Physical Description: Cryst.

Melting Point: Mp 234-235°

References: