



>>Entry Name: (Acetato-*O*)phenylmercury, 9CI

Synonym(s): Phenylmercuric acetate, USAN. Acetoxyphenylmercury. Acetoxymcuribenzene. Maysan. Ceresol. Anticon. Contracept. Gynophen. Senomen

CAS Registry Number: 62-38-4

XA4140

PhHgOAc

Molecular Formula: C₈H₈HgO₂

Molecular Weight: 336.74

Accurate Mass: 338.023047

Percentage Composition: C 28.53%; H 2.39%; Hg 59.57%; O 9.50%

Use/Importance: Bactericide, fungicide, algicide, disinfectant, spermicide, etc. Pharmaceutical excipient (preservative). Reference material used in elemental microanalysis. Adds to dienes in presence of catalytic Pd(OAc)₂ or stoichiometric Pd(OAc)₄; undergoes Heck reaction, stoichiometric in presence of Pd(OAc)₂ and catalytic in presence of Pd and Cu salts; substitutes allyl halides in presence of LiPdCl₃; homocouples to biphenyl in presence of PdCl₂/Py; reacts with CO/MeOH in presence of Wilkinson's catalyst; couples with phenylethyne in presence of Pd^{II} → PhC≡CPh; reacts with NOCl or NOBr → PhNO

Physical Description: Needles (H₂O) or lustrous cryst.

Melting Point: Mp 146-147° (152°)

Hazard & Toxicity: Highly toxic orally; LD₅₀ (rat, orl) 22 mg/kg

Aldrich: P2712-7

Fluka: 79120

Sigma: P5554

References:

- Bruker, A.B. *et al.*, *Zh. Obshch. Khim.*, 1958, **28**, 2725, (*synth*)
Heck, R.F. *et al.*, *J.A.C.S.*, 1968, **90**, 5518; 5531; 1969, **91**, 6707, (*reactions*)
Hutzinger, O. *et al.*, *Int. J. Environ. Anal. Chem.*, 1971, **1**, 85, (*ms*)
Analyst (London), 1972, **97**, 740, (*microanal*)
Kamenar, B. *et al.*, *Inorg. Chim. Acta*, 1972, **6**, 191, (*cryst struct*)
Sens, M.A. *et al.*, *J. Magn. Reson.*, 1975, **19**, 323, (*Hg-199 nmr*)
Brown, A.J. *et al.*, *J.C.S. Dalton*, 1976, 1589, (*cmr*)
Kretchmer, R.A. *et al.*, *J.O.C.*, 1976, **41**, 2661, (*homocoupling*)
Goggin, P.L. *et al.*, *J. Chem. Res., Synop.*, 1978, 171, (*ir, Raman*)
Schwartzman, G., *J. Pharm. Sci.*, 1978, **67**, 539, (*uv, ir*)
Fedorov, L.A. *et al.*, *J. Struct. Chem. (Engl. Transl.)*, 1978, **19**, 549, (*pmr*)
Michel, E. *et al.*, *J. Organomet. Chem.*, 1981, **204**, 1, (*cmr, Hg-199 nmr*)
Kamenar, B. *et al.*, *Croat. Chem. Acta*, 1984, **57**, 145; *CA*, **100**, 165859, (*cryst struct*)
Masucci, J.A. *et al.*, *Org. Mass Spectrom.*, 1987, **22**, 233, (*ms*)
Pesticide Manual, 9th edn., 1991, No. 9580
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al.*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 342-343
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1142
Hazards in the Chemical Laboratory, 3rd edn., (ed. Bretherick, L.), Royal Society of Chemistry, 1981, 382
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, ABU500