



>>Entry Name: Copper(I) trifluoromethanesulfonate

Synonym(s): Trifluoromethanesulfonic acid copper(I+) salt, 9Cl. Cuprous triflate. (Trifluoromethanesulfonato)copper

CAS Registry Number: 42152-44-3

CuOSO2CF3

Molecular Formula: CCuF3O3S

Molecular Weight: 212.616

Accurate Mass: 211.891622

Percentage Composition: C 5.65%; Cu 29.89%; F 26.81%; O 22.58%; S 15.08%

Source/Synthesis: Generated *in situ* from Cu(OTf)2 and diazo compds.

Use/Importance: Catalyst for alkene dimerisation and photocycloadditions, cyclopropanation and carbene addn., for promotion of Grob-type fragmentations and in Ullmann reactions. Used to separate alkenes (e.g. ethene) from other hydrocarbons, and CO. Complexes C6H6 and a range of polyenes. Activates C-H bonds in alkynes. Reagent for mild dehydration of alcohols

Physical Description: Air- and moisture-sensitive

>>Derivative: CO complex

CAS Registry Number: 81967-72-8

Molecular Formula: C2CuF3O4S

Molecular Weight: 240.627

Accurate Mass: 239.886537

Percentage Composition: C 9.98%; Cu 26.41%; F 23.69%; O 26.60%; S 13.33%

Physical Description: Near white (v. pale pink) microcryst.

Solubility: Sol. Et2O

Other Data: Stable indefinitely under CO. Limited air stability. Forms complexes with phen., bipy, TMED. Phosphines displace CO. Ir ν_{CO} 2118 cm^{-1}

>>Derivative: Cyclohexene complex (1:1)

Synonym(s): Cyclohexene copper trifluoromethanesulfonate

Molecular Formula: C7H10CuF3O3S

Molecular Weight: 294.761

Accurate Mass: 293.969872

Percentage Composition: C 28.52%; H 3.42%; Cu 21.56%; F 19.34%; O 16.28%; S 10.88%

Use/Importance: Possible catalyst in photochemically-induced alkene rearrangements

Physical Description: White cryst.

Solubility: Sol. toluene

>>Derivative: C6H6 complex (1:1)

CAS Registry Number: 42152-46-5

Molecular Formula: C7H6CuF3O3S

Molecular Weight: 290.73

Accurate Mass: 289.938572

Percentage Composition: C 28.92%; H 2.08%; Cu 21.86%; F 19.60%; O 16.51%; S 11.03%

Melting Point: Fp 7°

Aldrich: 40724-0

Fluka: 61255

References:

U.S. Pat., 1971, 3 763 200; *CA*, **80**, 70278x, (use)

Dines, M.B. *et al.*, *Chem. Comm.*, 1973, 12, (deriv, cryst struct)

Salomon, R.G. *et al.*, *J.A.C.S.*, 1973, **95**, 1889-1897; 1979, **101**, 3961-3963, (synth, derivs, use)

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1975, **5**, 151; 1977, **6**, 130; 1979, **7**, 76; 1980, **8**, 125; 1982, **10**, 108; 1984, **11**, 142

Masamune, S. *et al.*, *J.A.C.S.*, 1977, **99**, 6756-6758, (use)

Evers, J.Th.M. *et al.*, *Tet. Lett.*, 1978, 821-824; 2317-2320; 2321-2324, (use)

Nagayoshi, K.G. *et al.*, *Chem. Lett.*, 1983, 1355-1356, (use)

Doyle, G. *et al.*, *Inorg. Chem.*, 1983, **22**, 2892-2895, (CO complex)

Timmermans, P.J.J.A., *Tet. Lett.*, 1983, **24**, 1419-1422, (use)

Hefner, J.G. *et al.*, *J. Organomet. Chem.*, 1984, **260**, 369-380, (use)

Timmermans, P.J.J.A. *et al.*, *J. Organomet. Chem.*, 1984, **276**, 287-295, (cyclohexene complex, cryst struct)

Avasthi, K. *et al.*, *J.O.C.*, 1984, **49**, 4322-4324, (use)

Salomon, R.G. *et al.*, *Tet. Lett.*, 1984, **24**, 3167-3170, (use)

Laali, K. *et al.*, *Helv. Chim. Acta*, 1987, **70**, 607-611, (use)

Stang, P.J. *et al.*, *J.A.C.S.*, 1987, **109**, 228-235, (use)

Ghosh, S. *et al.*, *J.O.C.*, 1987, **52**, 83-90, (use)

Org. Synth., *Coll. Vol.*, 6, 1988, 737-744, (synth, use)

Encyclopaedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **2**, 1370, (synth, use)