



>>Entry Name: Tris(trifluoromethanesulfonato)scandium

Synonym(s): Scandium trifluoromethanesulfonate. Scandium triflate

CAS Registry Number: 144026-79-9



Molecular Formula: $\text{C}_3\text{F}_9\text{O}_9\text{S}_3\text{Sc}$

Molecular Weight: 492.167

Accurate Mass: 491.811986

Percentage Composition: C 7.32%; F 34.74%; O 29.26%; S 19.55%; Sc 9.13%

Source/Synthesis: Synth. from $\text{ScCl}_3 \cdot x\text{H}_2\text{O}$ and $\text{F}_3\text{CSO}_3\text{H}$, followed by dehydration *in vacuo* at 200°

Use/Importance: Important water-soluble reusable Lewis acid catalyst in whole range of org. reactions. Catalyses allylation of carbonyl compds. with $\text{Sn}(\text{C}_3\text{H}_5)_4$; Diels-Alder catalyst; catalyses aldol and Michael reactions of silyl enolates; catalyst in synth. of chiral acetals; catalyses alkylation of aromatics by alkenes; catalyst for acylaminoalkylation and Friedel-Crafts alkylation reactions; catalyst for Friedel-Crafts benzylation and alkylation of aromatics. In presence of surfactants, catalyses aldol synth., synth. of homoallylic alcohols and homoallylic amines. Catalyst for one-pot synth. of pyrroline and quinoline derivs; catalyst for reactions of imines; catalyst for synth. of enamine derivs.

Physical Description: Grey solid

Solubility: Sol. H_2O

Aldrich: 41821-8

Fluka: 84645

>>Derivative: Nonahydrate

Synonym(s): Nonaaquascandium(3+) tris(trifluoromethanesulfonate)

Molecular Formula: $\text{C}_3\text{H}_{18}\text{F}_9\text{O}_{18}\text{S}_3\text{Sc}$

Molecular Weight: 654.304

Percentage Composition: C 5.51%; H 2.77%; F 26.13%; O 44.01%; S 14.70%; Sc 6.87%

Source/Synthesis: Synth. by refluxing 1M $\text{F}_3\text{CSO}_3\text{H}$ with Sc_2O_3 until neutral

Physical Description: White cryst.

Solubility: Sol. H_2O

Other Data: Contains trigonal prismatic $[\text{Sc}(\text{OH}_2)_9]^{3(+)}$; isomorphous with La-Lu, Y analogues

References:

- Hachiya, I. *et al.*, *J.O.C.*, 1993, **58**, 6958, (*use, allylation of carbonyl compds*)
Kobayashi, S. *et al.*, *Synlett*, 1993, 462, (*use, Diels-Alder, aldol, Michael reactions of silyl enolates*)
Kobayashi, S. *et al.*, *Tet. Lett.*, 1993, **34**, 3755, (*use, Michael addn, Diels-Alder catalyst*)
Hamidi, M.E.M. *et al.*, *Polyhedron*, 1994, **13**, 1787, (*synth, ir*)
Kawada, A. *et al.*, *Synlett*, 1994, 545, (*use, acylation of benzene derivs*)
Kobayashi, S., *Synlett*, 1994, 689, (*use, rev*)
Kobayashi, S. *et al.*, *Chem. Lett.*, 1995, 423, (*use, synth of pyrroline and quinoline derivs*)
Castellani, C.B. *et al.*, *Eur. J. Solid State Inorg. Chem.*, 1995, **32**, 1089, (*nonahydrate, synth, cryst struct*)
Ishihara, K. *et al.*, *J.A.C.S.*, 1995, **117**, 4413, (*use, acylation*)
Japan. Pat., 1995, 072 58116; *CA*, 1996, **124**, 116843, (*use, alkylation of aromatics*)
Fukuzawa, S. *et al.*, *Synlett*, 1995, 1077, (*use, chiral acetal synth*)
Bellucci, C. *et al.*, *Tet. Lett.*, 1995, **36**, 7289, (*use, reactions of imines*)
Tsuchimoto, T. *et al.*, *Chem. Comm.*, 1996, 2344, (*use, benzylation of aromatics*)
Ishitani, H. *et al.*, *J.O.C.*, 1996, **61**, 1902, (*use, reactions of imines*)
Ishihara, K. *et al.*, *J.O.C.*, 1996, **61**, 4560, (*use, acylation*)
Tsuchimoto, T. *et al.*, *Synlett*, 1996, 557, (*use, Friedel-Crafts benzylation and allylation of aromatics*)
Ishihara, K. *et al.*, *Synlett*, 1996, 839, (*use, chiral acetal synth*)
El Gihami, M.T. *et al.*, *Synlett*, 1996, 871, (*use, acylaminoalkylation and Friedel-Crafts alkylations*)
Kobayashi, S. *et al.*, *Synlett*, 1996, 1153, (*use, acylation of phenols and naphthols*)
Jenner, G. *et al.*, *Tet. Lett.*, 1996, **37**, 3691, (*use, enamine synth*)
Barrett, A.G.M. *et al.*, *Chem. Comm.*, 1997, 351, (*use, acylation of alcohols*)
Waller, F.J. *et al.*, *Chem. Comm.*, 1997, 613, (*use, nitration*)
Kobayashi, S. *et al.*, *Chem. Lett.*, 1997, 831, (*use, synth of homoallylic alcohols*)
Kobayashi, S. *et al.*, *Tet. Lett.*, 1997, 4559, (*use, aldol synth*)
Kobayashi, S. *et al.*, *Chem. Comm.*, 1998, 19, (*use, synth of homoallylic amines*)
Kobayashi, S. *et al.*, *Chem. Comm.*, 1998, 19-20, (*use*)