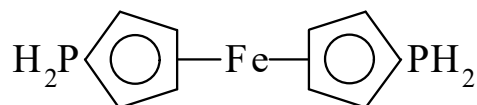




>>Entry Name: 1,1'-Diphosphinoferrocene



Related CAS Registry Numbers(s): 95408-37-0 95464-04-3

Molecular Formula: $C_{10}H_{12}FeP_2$

Molecular Weight: 249.999

Accurate Mass: 249.976363

Percentage Composition: C 48.04%; H 4.84%; Fe 22.34%; P 24.78%

>>Derivative: *P,P'*-Tetra-Me

Synonym(s): 1,1'-Bis(dimethylphosphino)ferrocene, 9Cl

CAS Registry Number: 32680-64-1

Molecular Formula: $C_{14}H_{20}FeP_2$

Molecular Weight: 306.106

Accurate Mass: 306.038963

Percentage Composition: C 54.93%; H 6.59%; Fe 18.24%; P 20.24%

Source/Synthesis: Synth. from $FeCp_2$ and BuLi/TMED, then Me_2PCl

Physical Description: Air-sensitive dark red oil

Boiling Point: $Bp_{0.05}$ 104-108°

>>Derivative: *P,P'*-Tetra-*tert*-butyl

Synonym(s): 1,1'-Bis(di-*tert*-butylphosphino)ferrocene

CAS Registry Number: 84680-95-5

Molecular Formula: $C_{26}H_{44}FeP_2$

Molecular Weight: 474.428

Accurate Mass: 474.226763

Percentage Composition: C 65.82%; H 9.35%; Fe 11.77%; P 13.06%

Source/Synthesis: Synth. from $Fe(C_5H_4Li)_2$ /TMED + Bu^t_2PCl

Physical Description: Dark orange oil

Other Data: Dec. at 153-155°

>>Derivative: *P,P'*-Di-*tert*-butyl-di-Ph

Synonym(s): 1,1'-Bis[(1,1-dimethylethyl)phenylphosphino]ferrocene, 10Cl

Molecular Formula: $C_{30}H_{36}FeP_2$

Molecular Weight: 514.409

Accurate Mass: 514.164163

Percentage Composition: C 70.05%; H 7.05%; Fe 10.86%; P 12.04%

Source/Synthesis: Synth. from $Fe(C_5H_4Li)_2$ + Bu^tPPhCl

Physical Description: Deep red solid

Melting Point: Mp 56-58°

Other Data: The *meso* and racemic isomers can be sepd. by chromatog. Rh complexes have also been reported

>>Derivative: *P,P'*-Tetrafluoro

Synonym(s): 1,1'-Bis(difluorophosphino)ferrocene, 12Cl

CAS Registry Number: 126481-15-0

Molecular Formula: $C_{10}H_8F_4FeP_2$

Molecular Weight: 321.961

Accurate Mass: 321.938675

Percentage Composition: C 37.31%; H 2.50%; F 23.60%; Fe 17.35%; P 19.24%

Source/Synthesis: Synth. from $Fe(C_5H_4Li)_2$ + PF_2Cl

>>Derivative: *P,P'*-Tetra-Ph

see 1,1'-Bis(diphenylphosphino)ferrocene, [JLG23-E](#)

References:

- Bishop, J.J. *et al.*, *J. Organomet. Chem.*, 1971, **27**, 241, (*tetra-Me*, synth, pmr, ir)
Cullen, W.R. *et al.*, *Organometallics*, 1983, **2**, 714, (*tetra-tert-butyl*, synth, struct, pmr)
Einstein, F.W.B. *et al.*, *Acta Cryst. C*, 1985, **41**, 365, (*di-tert-butyl-di-Ph*, cryst struct, Rh complexes)
Butler, I.R. *et al.*, *Organometallics*, 1985, **4**, 972, (*di-tert-butyl-di-Ph*, synth, pmr)
Hever, L. *et al.*, *Z. Naturforsch., B*, 1989, **44**, 1082, (*tetrafluoro*, synth, pmr)