

ISOPROPYL METHYL METHYLTHIOPHOSPHONATE

CAS RN 38315-92-3 (S), 38315-91-2 (R)

14-3-1

Instrument: Bruker AC-250
Nucleus: ¹H
Frequency: 250.13 Hz

Solvent: CDCl₃
Concentration: 21 mg/ml
Temperature: 23°C
Reference: TMS (int.)
Spectral width: 2873.6 Hz
Pulse width: 4.7 μs (45°)
Repetition time: 12.4 s
Data points
FID/Spectrum: 64 K/64 K
Scans: 64
Line broadening: 0.05 Hz (exp.)
Resolution: 0.8 Hz (TMS)

Assignments

a,a': δ = 1.30(d), 1.31(d);
J_{a-d} = J_{a'-d} = 6.2 Hz
b: δ = 1.79(d); J_{b-p} = 15.5 Hz
c: δ = 3.69(d); J_{c-p} = 13.9 Hz
d: δ = 4.82(d, sept.);
J_{d-p} = 11.2 Hz,
J_{d-a} = 6.2 Hz

