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tert-Butylfluorodiphenylsilane

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.003 Å
R factor = 0.038
wR factor = 0.095
Data-to-parameter ratio = 20.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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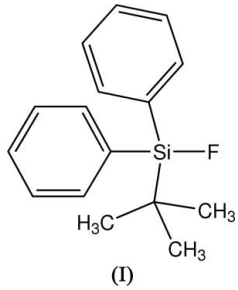
In the title compound, $C_{16}H_{19}FSi$, the Si atom approximates the expected tetrahedral geometry, with an Si—F bond length of 1.6004 (10) Å.

Comment

In the title compound, (I), the Si atom shows a slightly distorted tetrahedral configuration, with bond angles ranging from 105.43 (6) (F1—Si1—C21) to 113.69 (7)° (C1—Si1—C21). The Si1—F1 bond length of 1.6004 (10) Å is as expected and is comparable with that in fluorotri-*o*-tolylsilane [Si—F = 1.601 (1) Å at 298 K; Dell *et al.*, 1999].



(I)

Experimental

The synthesis of (I) will be described elsewhere (Schirrmacher *et al.*, 2006). In contrast to earlier findings (Damrauer *et al.*, 1988), compound (I) crystallized spontaneously from the melt after it had been distilled *in vacuo*.

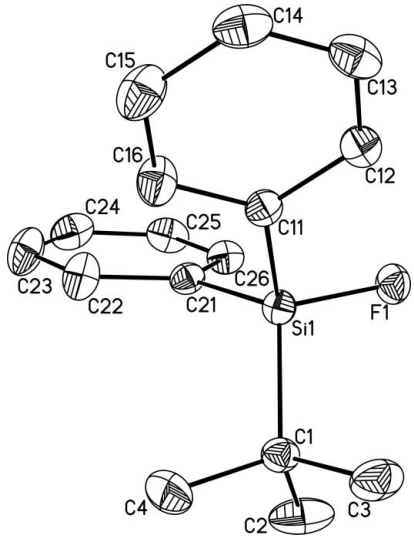


Figure 1
View of (I), showing the labelling scheme and displacement ellipsoids drawn at the 30% probability level. H atoms have been omitted.

Crystal data

$C_{16}H_{19}FSi$	D_x = 1.166 Mg m^{-3}
M_r = 258.40	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 14895 reflections
a = 9.5029 (8) Å	θ = 2.9–27.5°
b = 22.984 (2) Å	μ = 0.15 mm^{-1}
c = 7.2776 (5) Å	T = 173 (1) K
β = 112.226 (5)°	Block, colourless
V = 1471.4 (2) Å^3	0.26 × 0.24 × 0.24 mm
Z = 4	

Data collection

Nonius KappaCCD diffractometer	R_{int} = 0.048
ω scans	θ_{max} = 27.5°
Absorption correction: none	$h = -12 \rightarrow 11$
14895 measured reflections	$k = -29 \rightarrow 29$
3366 independent reflections	$l = -9 \rightarrow 9$
1836 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.038	$w = 1/[\sigma^2(F_o^2) + (0.0518P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.095	$(\Delta/\sigma)_{max} < 0.001$
S = 0.80	$\Delta\rho_{max}$ = 0.26 e Å^{-3}
3366 reflections	$\Delta\rho_{min}$ = −0.18 e Å^{-3}
166 parameters	

All H atoms were placed in calculated positions and refined using a riding model, with $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl groups and $U_{iso} = 1.2U_{eq}(C)$ for aryl groups. The methyl groups were allowed to rotate but not to tip. Constrained CH bond lengths: 0.93 Å for aryl CH and 0.96 Å for methyl CH_3.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

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