scheme are shown in Fig. 1 and a stereoscopic view in Fig. 2. Positional parameters and the equivalent values of the anisotropic temperature factors for the non-H atoms are given in Table 1.* Bond lengths and angles are given in Table 2.

Related literature. Babichev, Kovtunenko & Tyltin (1981), Bonnett, Hursthouse, North & Trotter (1985), Kohl (1984), Kreher (1986), Kovtunenko *et al.* (1984).

* Lists of H-atom coordinates, anisotropic thermal parameters and structure-factor amplitudes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44866 (7 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

BABICHEV, F. S., KOVTUNENKO, V. A. & TYLTIN, A. K. (1981). *Usp. Khim.* **50**, 2073–2105 (Russian edition); *Russ. Chem. Rev.* **50**, 1087–1103 (English edition).

BONNETT, R., HURSTHOUSE, M. B., NORTH, S. A. & TROTTER, J. (1985). *J. Chem. Soc. Perkin Trans.* 2, pp. 293–296.

FRENZ, B. A. (1985). *Enraf–Nonius SDP-Plus Structure Determination Package*, version 3.0. Enraf–Nonius, Delft, The Netherlands.

International Tables for X-ray Crystallography (1974). Vol. IV, Tables 2.2B and 2.3.1. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)

KOHL, N. (1984). Dissertation, Univ. Dortmund, Federal Republic of Germany.

KOVTUNENKO, V. A., VOITENKO, Z. V., CHERNEGA, A. N., ESPENBETOV, A. A., ANTIPIN, M. YU., TYLTIN, A. K., STRUCHKOV, YU. T. & BABICHEV, F. S. (1984). *Ukr. Khim. Zh.* (*Russ. Ed.*), **50**, 988–991; *Chem Abstr.* (1985), **102**, 24424s.

KREHER, R. P. (1986). *Univ.-Rep. Univ. Dortmund*, **3**, 2–3.

MAIN, P., FISKE, S. J., HULL, S. E., LESSINGER, L. GERMAIN, G., DECLERCQ, J.-P. & WOOLFSON, M. M. (1980). *MULTAN80. A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data.* Univs. of York, England, and Louvain, Belgium.

NARDELLI, M. (1983). *Comput. Chem.* **7**, 95–98.

SHELDRICK, G. M. (1987). *SHELXTL-Plus*, release 2. *An Integrated System for Solving, Refining and Displaying Crystal Structures from Diffraction Data.* For Nicolet *R3m/V*. Univ. of Göttingen, Federal Republic of Germany.

Acta Cryst. (1988). C**44**, 1323–1324

Ethyl 3-(2-Methyl-1,3-dioxolan-2-yl)-2-(methyldiphenylsilyl)propionate

BY CHARLES L. BARNES, GERALD L. LARSON,* ANGEL SANTIAGO AND JORGE RIOS STEINER

Department of Chemistry, University of Puerto Rico, Rio Piedras, PR 00931, *USA*

(*Received* 7 *December* 1987; *accepted* 19 *February* 1988)

Abstract. $C_{22}H_{28}O_4Si$, $M_r = 384{\cdot}5$, triclinic, $P\bar{1}$, $a = 9{\cdot}633$ (3), $b = 10{\cdot}010$ (3), $c = 12{\cdot}790$ (4) Å, $\alpha = 106{\cdot}15$ (10), $\beta = 105{\cdot}72$ (11), $\gamma = 101{\cdot}16$ (15)°, $V = 1091$ (1) Å^3, $Z = 2$, $D_m = 1{\cdot}167$, $D_x = 1{\cdot}170$ g cm^{-3}, λ(Cu $K\bar{\alpha}$) = 1·5418 Å, $\mu = 11{\cdot}2$ cm^{-1}, $F(000) = 412$, $T = 297$ K, $R = 0{\cdot}056$ for 3956 observed reflections (of 4478 unique data). Si–C distances are 1·876 (2) and 1·873 (2) Å (phenyl), 1·865 (2) Å methyl) and 1·903 (2) Å (propionate). No evidence for and interaction between the Si atom and the carbonyl O atom was found.

Experimental. Colorless crystal, dimensions 0·25 × 0·32 × 0·35 mm, mounted on a glass fiber, space group from successful refinement of centrosymmetric model, cell dimensions from setting angles for 25 reflections having $36 < \theta < 45°$. Data collection on Enraf–Nonius CAD-4 diffractometer, Cu $K\bar{\alpha}$ radiation, graphite monochromator, ω–2θ scans at 2·1 to 16·5° min^{-1}. Data having $2\theta \le 150°$, $0 \le h \le 12$, $-12 \le k \le 12$, $-15 \le l \le 14$ measured. Three standard reflections ($3\bar{2}9$, $0\bar{4}\bar{7}$, $\bar{3}2\bar{9}$) measured every 3600s, maximum variation 3·6%. 4478 unique data, 3956 reflections with $I > 3\sigma(I)$ considered observed, corrected for background, Lorentz, polarization, no absorption correction applied. Solved by direct methods using *MULTAN*11/82 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1982) and Fourier methods. Full-matrix least-squares methods minimized $\sum w(|F_o| - |F_c|)^2$ with $w = 4F_o^2[\sigma^2(I) + (0{\cdot}05F_o^2)^2]^{-1}$. Non-H atoms refined with anisotropic thermal parameters, H atoms placed at calculated positions and not refined. Final $R = 0{\cdot}056$, $wR = 0{\cdot}090$, $S = 2{\cdot}52$, for observed data. Max. $\Delta/\sigma = 0{\cdot}01$ in final cycle, max. residual density 0·24 e Å^{-3}. An empirical extinction correction was applied: $F^{corr} = F_c/(1 + 1{\cdot}0 \times 10^{-6}F_c^2\text{Lp})$, where Lp is the Lorentz–polarization correction factor. Atomic scattering factors and anomalous-dispersion corrections from *International Tables for X-ray Crystal-*

* Current address: Petrarch Systems, Bartram Road, Bristol, PA 19007, USA.

0108-2701/88/071323-02$03.00

lography (1974) and programs used were those of Enraf–Nonius (1982) *SDP*. Table 1 gives the atom coordinates and molecular dimensions are given in Table 2.* Fig. 1 (*ORTEP*; Johnson, 1976) shows the molecular structure and numbering scheme.

* Lists of H-atom parameters, anisotropic thermal parameters and structure-factor amplitudes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44796 (48 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters*

	x	y	z	B_{eq}(Å^2)
Si	0·10735 (5)	0·26108 (5)	0·77589 (4)	3·94 (1)
O1	0·3296 (2)	0·1723 (2)	0·9832 (1)	6·76 (5)
O2	0·4064 (2)	0·1076 (2)	0·8318 (1)	5·79 (4)
O3	0·1569 (2)	−0·1779 (2)	0·8438 (1)	6·40 (4)
O4	−0·0086 (2)	−0·2197 (1)	0·6672 (1)	4·98 (3)
C1	0·3021 (2)	0·1259 (2)	0·8805 (2)	4·52 (4)
C2	0·1493 (2)	0·0879 (2)	0·7908 (1)	3·79 (3)
C3	0·0267 (2)	−0·0007 (2)	0·8199 (1)	4·19 (4)
C4	0·0165 (2)	−0·1612 (2)	0·7874 (2)	4·40 (4)
C5	−0·1080 (3)	−0·2446 (3)	0·8160 (2)	7·66 (6)
C6	0·5606 (3)	0·1479 (4)	0·9132 (3)	8·6 (1)
C7	0·6535 (4)	0·1018 (8)	0·8500 (4)	16·3 (2)
C8	0·2020 (3)	−0·2666 (3)	0·7612 (4)	9·5 (1)
C9	0·0811 (3)	−0·3140 (3)	0·6506 (2)	6·90 (6)
C10	0·2519 (2)	0·3604 (2)	0·7295 (2)	3·97 (4)
C11	0·3884 (2)	0·4556 (2)	0·8074 (2)	5·07 (5)
C12	0·4913 (2)	0·5350 (3)	0·7733 (2)	6·01 (6)
C13	0·4568 (2)	0·5194 (3)	0·6576 (2)	6·04 (5)
C14	0·3226 (3)	0·4246 (3)	0·5781 (2)	5·90 (5)
C15	0·2208 (2)	0·3464 (2)	0·6134 (2)	4·76 (4)
C16	−0·0823 (2)	0·2065 (2)	0·6610 (2)	4·41 (4)
C17	−0·1417 (2)	0·0743 (3)	0·5694 (2)	5·34 (5)
C18	−0·2794 (3)	0·0388 (3)	0·4831 (2)	6·54 (6)
C19	−0·3632 (3)	0·1343 (3)	0·4862 (3)	7·58 (7)
C20	−0·3090 (3)	0·2644 (3)	0·5747 (3)	8·57 (8)
C21	−0·1704 (3)	0·3017 (2)	0·6618 (2)	6·58 (6)
C22	0·1075 (3)	0·3813 (2)	0·9165 (2)	6·16 (5)

Anisotropically refined atoms are given in the form of the equivalent isotropic displacement parameter defined as:

$\frac{4}{3}[a^2B(1,1) + b^2B(2,2) + c^2B(3,3) + ab(\cos\gamma)B(1,2) + ac(\cos\beta)B(1,3) + bc(\cos\alpha)B(2,3)]$.

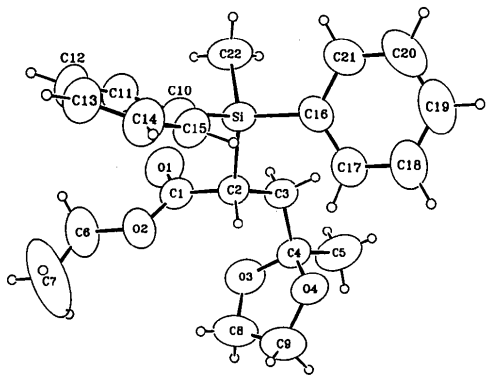

Fig. 1. Perspective view of the molecule with numbering scheme. Thermal ellipsoids are drawn at the 50% probability level.

Table 2. *Bond lengths* (Å) *and angles* (°) *with e.s.d.'s in parentheses*

Si–C2	1·903 (2)	C6–C7	1·418 (6)
Si–C10	1·876 (2)	C8–C9	1·449 (4)
Si–C16	1·873 (2)	C10–C11	1·381 (2)
Si–C22	1·865 (2)	C10–C15	1·393 (3)
O1–C1	1·199 (3)	C11–C12	1·388 (4)
O2–C1	1·333 (3)	C12–C13	1·381 (4)
O2–C6	1·466 (3)	C13–C14	1·372 (3)
O3–C4	1·416 (3)	C14–C15	1·384 (3)
O3–C8	1·403 (4)	C16–C17	1·390 (2)
O4–C4	1·417 (2)	C16–C21	1·393 (3)
O4–C9	1·409 (3)	C17–C18	1·382 (3)
C1–C2	1·500 (2)	C18–C19	1·365 (5)
C2–C3	1·528 (3)	C19–C20	1·358 (4)
C3–C4	1·519 (3)	C20–C21	1·390 (4)
C4–C5	1·513 (4)		

C2–Si–C10	110·17 (9)	C3–C4–C5	112·0 (2)
C2–Si–C16	107·43 (7)	O2–C6–C7	108·6 (3)
C2–Si–C22	110·3 (1)	O3–C8–C9	107·0 (3)
C10–Si–C16	108·91 (9)	O4–C9–C8	105·0 (2)
C10–Si–C22	109·57 (9)	Si–C10–C11	122·6 (2)
C16–Si–C22	110·5 (1)	Si–C10–C15	120·3 (1)
C1–O2–C6	115·3 (2)	C11–C10–C15	117·0 (2)
C4–O3–C8	109·1 (2)	C10–C11–C12	122·3 (2)
C4–O4–C9	108·4 (2)	C11–C12–C13	119·3 (2)
O1–C1–O2	123·6 (2)	C12–C13–C14	119·6 (2)
O1–C1–C2	124·9 (2)	C13–C14–C15	120·4 (2)
O2–C1–C2	111·5 (2)	C10–C15–C14	121·3 (1)
Si–C2–C1	109·4 (1)	Si–C16–C17	123·4 (2)
Si–C2–C3	111·2 (1)	Si–C16–C21	120·4 (1)
C1–C2–C3	111·7 (2)	C17–C16–C21	116·1 (2)
C2–C3–C4	114·0 (2)	C16–C17–C18	122·4 (2)
O3–C4–O4	105·5 (2)	C17–C18–C19	120·1 (2)
O3–C4–C3	109·8 (1)	C18–C19–C20	119·1 (2)
O3–C4–C5	110·6 (2)	C19–C20–C21	121·3 (3)
O4–C4–C3	108·8 (2)	C16–C21–C20	120·9 (2)
O4–C4–C5	110·0 (1)		

Related literature. Larson (1984); Larson & Betancourt de Perez (1985); Larson, Hernandez, Montes de Lopez-Cepero & Torres (1985); Larson, Santiago & Montes de Lopez-Cepero (1986*a*,*b*).

References

Enraf–Nonius (1982). *Structure Determination Package.* Enraf–Nonius, Delft, The Netherlands.

International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)

JOHNSON, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.

LARSON, G. L. (1984). *Silicon Compounds: Register and Review,* pp. 22–32. Petrarch Systems Inc., Bristol, PA, USA.

LARSON, G. L. & BETANCOURT DE PEREZ, R. M. (1985). *J. Org. Chem.* **50**, 5257–5260.

LARSON, G. L., HERNANDEZ, D., MONTES DE LOPEZ-CEPERO, I. & TORRES, L. E. (1985). *J. Org. Chem.* **50**, 5260–5267.

LARSON, G. L., SANTIAGO, A. & MONTES DE LOPEZ-CEPERO, I. (1986*a*). *Synth. Commun.* **16**, 697–704.

LARSON, G. L., SANTIAGO, A. & MONTES DE LOPEZ-CEPERO, I. (1986*b*). *Synth. Commun.* **16**, 705–711.

MAIN, P., FISKE, S. J., HULL, S. E., LESSINGER, L., GERMAIN, G., DECLERCQ, J.-P. & WOOLFSON, M. M. (1982). *MULTAN*11/82. *A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data.* Univs. of York, England, and Louvain, Belgium.