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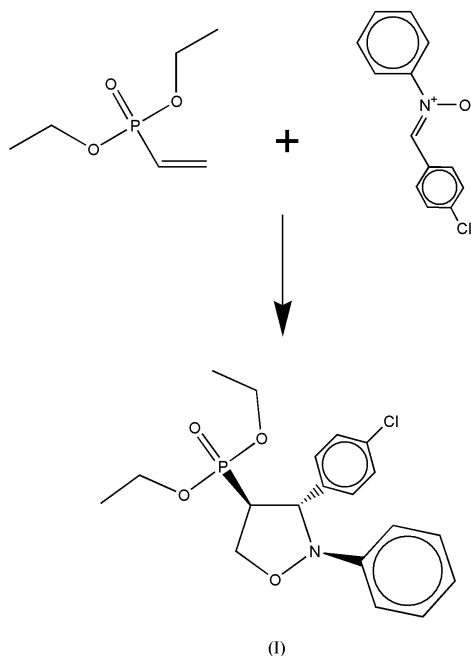
Key indicators

Single-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.008\text{ \AA}$
Disorder in main residue
 R factor = 0.070
 wR factor = 0.211
Data-to-parameter ratio = 13.1For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.3-(4-Chlorophenyl)-4-(*O,O'*-diethylphosphono)-2-phenylisoxazolidine

The title compound, $\text{C}_{19}\text{H}_{23}\text{ClNO}_4\text{P}$, is a novel heterocyclic compound which can be synthesized by the reaction of a vinyl phosphonate with a nitron. The phenyl and chlorophenyl rings lie on opposite sides of the isoxazolidine ring, which adopts a twist conformation.

Comment

In the title compound, (I), the phenyl and chlorophenyl rings lie on opposite sides of the isoxazolidine ring, which adopts a twist conformation. The dihedral angle between the two six-membered rings is $54.7(2)^\circ$.



The geometry of the heterocyclic ring is similar to that found in (+)-(3*R*,5*S*)-3-(4-chlorophenyl)-5-ethoxy-2-phenylisoxazolidine (Simonsen *et al.*, 1999), 5-acetoxy-2,3-diphenylisoxazolidine and 5-acetoxy-3-(4-nitrophenyl)-2-phenylisoxazolidine (Mukherjee *et al.*, 1999).

The geometry of the phosphonate group has been compared with those found in four other phosphonate structures: diethyl (*N*-hydroxy-2-methylpyrrolidin-2-yl)phosphonate (Barbati *et al.*, 1997), diethyl 5,6-dihydro-2*H*-1,3-dithiolo[4,5-*b*][1,4]dithiin-2-ylphosphonate (Kelkar *et al.*, 1994), (2'*S*,3'*S*,4'*R*)-5'-*O*-benzoyl-3'-deoxy-3' β -diethylphosphono-2'-*O*-*tert*-butyldimethylsilyluridine (McEldoon *et al.*, 1996) and diethyl (1-hydroxy-2-butynyl)phosphonate (Sanders *et al.*, 1996). For these four structures, the average bond lengths are: $\text{P}-\text{C} = 1.810\text{ \AA}$, $\text{P}-\text{O} = 1.569\text{ \AA}$ and $\text{P}=\text{O}$

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= 1.465 Å. The corresponding values in the title compound are markedly different, *viz.* 1.776 (5), 1.544 (4)/1.590(5) and 1.419 (5) Å, respectively. In the title compound, the P atom adopts a distorted tetrahedral configuration, with angles in the range 101.9 (2)–117.0 (3)°.

Experimental

To a solution of nitron (0.278g, 1.2 mmol) in 20 ml dried benzene was added vinyl phosphonate (0.164g, 1 mmol) and the resulting solution was heated under an N₂ atmosphere with reflux for 24 h. The reaction mixture was then cooled to room temperature and concentrated under reduced pressure. The title compound was obtained by column chromatography. Recrystallization from hexane and dichloroethane (4:1 *v/v*) afforded colorless crystals. Analysis calculated for C₁₉H₂₃ClNO₄P: C 57.65, H 5.86, N 3.54%; found: C 57.42, H 5.98, N 3.38%.

Crystal data

C₁₉H₂₃ClNO₄P
M_r = 395.80
 Monoclinic, *C2/c*
a = 24.02 (2) Å
b = 10.563 (9) Å
c = 16.410 (14) Å
 β = 100.900 (18)°
V = 4089 (6) Å³
Z = 8

D_x = 1.286 Mg m⁻³
 Mo *K*α radiation
 Cell parameters from 684 reflections
 θ = 3.2–19.3°
 μ = 0.29 mm⁻¹
T = 293 (2) K
 Block, colorless
 0.22 × 0.20 × 0.18 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Bruker, 2001)
T_{min} = 0.768, *T_{max}* = 0.949
 9919 measured reflections

3598 independent reflections
 1569 reflections with *I* > 2σ(*I*)
R_{int} = 0.070
 θ_{\max} = 25.0°
h = -17 → 28
k = -11 → 12
l = -19 → 16

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.070
wR (*F*²) = 0.211
S = 1.01
 3598 reflections
 274 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.091P)^2 + 2.6884P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.57 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -0.31 \text{ e } \text{Å}^{-3}$
 Extinction correction: SHELXL97
 Extinction coefficient: 0.0025 (5)

Table 1

Selected geometric parameters (Å, °).

P1–O2	1.419 (5)	N1–C1	1.496 (6)
P1–O4	1.544 (4)	O1–C3	1.422 (6)
P1–O3	1.590 (5)	C1–C2	1.550 (6)
P1–C2	1.776 (5)	C2–C3	1.514 (7)
N1–O1	1.447 (5)		
O2–P1–O4	114.4 (2)	C3–O1–N1	105.6 (3)
O2–P1–O3	117.0 (3)	N1–C1–C4	111.1 (3)
O4–P1–O3	102.6 (3)	N1–C1–C2	104.3 (3)
O2–P1–C2	113.9 (3)	C4–C1–C2	115.2 (4)
O4–P1–C2	105.4 (2)	C3–C2–C1	101.0 (4)
O3–P1–C2	101.9 (2)	C3–C2–P1	115.1 (3)
C10–N1–O1	111.5 (3)	C1–C2–P1	114.1 (3)
C10–N1–C1	117.6 (3)	O1–C3–C2	103.4 (4)
O1–N1–C1	107.0 (3)		

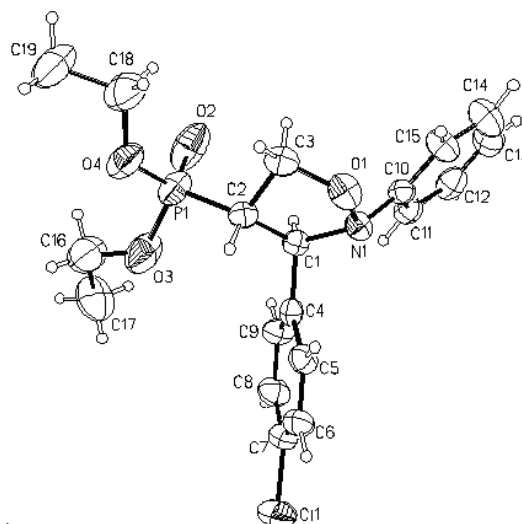


Figure 1

ORTEP-3 (Farrugia, 1997) plot of the title compound. Displacement ellipsoids are drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radii. Only the major disorder components are shown.

The H atoms were positioned geometrically, with C–H = 0.93, 0.98, 0.97 or 0.96 Å for phenyl, tertiary, methylene and methyl H atoms, respectively, and were included in the refinement in the riding-model approximation. For methyl H atoms, $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{carrier atom})$; for other H atoms $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{carrier atom})$. Both ethyl groups exhibit disorder over two positions, and a split model has been used. The site-occupancy factors have been refined to 0.728 (13):0.272 (13) for C16 and C17, and to 0.537 (14):0.463 (14) for C18 and C19.

Data collection: SMART (Bruker, 2001); cell refinement: SMART; data reduction: SAINT (Bruker, 2001); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 (Farrugia, 1997); software used to prepare material for publication: SHELXTL (Bruker, 2001).

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