2-(Diphenylphosphino)phenyl 2-(diphenylphosphinoyl)phenyl ether

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The title compound, \( \text{C}_{36}\text{H}_{28}\text{O}_{2}\text{P}_{2} \), features weak inter- and intramolecular hydrogen bonds linking molecules into infinite chains.

Comment

The title compound, (I), was inadvertently obtained during an attempt to synthesize a nickel–phosphine complex.

The structure features a weak hydrogen bond between aromatic atom H6 and the phosphine oxide O atom, which a search of the Cambridge Structural Database (Version 5.26; Allen, 2002) shows to be a common feature in phenyl-substituted phosphine oxides. An additional weak (Steiner, 1996) bifurcated intermolecular hydrogen bond is also present between O2 and H27 and H28, which joins the molecules into an infinite chain along [1\(\overline{1}\)0].

Figure 1

View of the title compound with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity.
Experimental

A tetrahydrofuran solution of 2 equivalents of bis[2-(diphenylphosphino)phenyl] ether and bis(1,5-cyclooctadiene)nickel(0) was layered with n-pentane and placed in a freezer, resulting in a crop of off-white crystals after 5 d. $^{31}$P NMR (162 MHz, C₆D₆): δ 22.8 (s), −17.5 (s).

Crystal data

C₃₆H₂₈O₂P₂
Mr = 554.52
Triclinic, P

a = 9.9316 (7) Å
b = 10.2786 (5) Å
c = 14.5778 (10) Å

α = 75.785 (4)°
β = 83.778 (6)°
γ = 85.529 (6)°

V = 1432.05 (16) Å³

Z = 2

D = 1.286 Mg m⁻³

Cell parameters from 152 reflections

θ = 4.3–21.9°
μ = 0.18 mm⁻¹

T = 150 (2) K

Block, colourless

0.3 × 0.3 × 0.15 mm

Data collection

Nonius KappaCCD diffractometer
ω and φ scans
Absorption correction: none

26296 measured reflections
6527 independent reflections
5195 reflections with I > 2σ(I)

Refinement

Refinement on F²
R[F² > 2σ(F²)] = 0.039
wR(F²) = 0.098
S = 1.04

6527 reflections
361 parameters
H-atom parameters constrained

w = 1/[σ²(Fo)² + (0.0396P)² + 0.7162P]

R[Fo] = 0.044
θ(max) = 27.5°

C6—H6···O2 0.95 2.56 2.975 (2) 107
C27—H27···O2 0.95 2.59 3.206 (2) 123
C28—H28···O2 0.95 2.58 3.202 (2) 123

Symmetry code: (i) x + 1, y + 1, z.

Table 1

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<tr>
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Data collection: COLLECT (Hooft, 1998); cell refinement: DIRAX (Duisenberg, 1992); data reduction: EVALCCD (Duisenberg et al., 2003); program(s) used to solve structure: SHELXS86 (Sheldrick, 1985); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: PLATON (Spek, 2003); software used to prepare material for publication: PLATON.

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References