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O-Pivaloyl diphenylselenophosphinate

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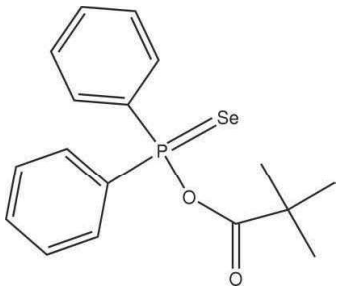
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.006 Å; R factor = 0.057; wR factor = 0.147; data-to-parameter ratio = 19.0.

The title compound, $C_{17}H_{19}O_2PSe$, was obtained in the reaction of the diphenylmonoselenophosphinic acid ammonium salt with pivaloyl chloride. The P—Se bond length of 2.0769 (11) Å is normal, while the P—O bond length of 1.650 (3) Å is longer than in related *O*-alkyl and *O*-aryl derivatives. One phenyl ring is periplanar to the Se—P—C plane, while the dihedral angle between the two phenyl rings is *ca* 73°. The carbonyl group is in a synperiplanar position [torsion angle = 8.9 (6)°] to one of the methyl groups of the pivaloyl group. This is the first *O*-acyl derivative of diphenylmonoselenophosphinic acid characterized by X-ray structural analysis.

Related literature

Syntheses and the chemical properties of *O*-acyl monoselenophosphates have already been described by Rachon *et al.* (2005). For other monoselenophosphates, such as *O*-alkyl or *O*-aryl esters, see: Lepicard *et al.* (1969); Balakrishna *et al.* (2002, 2005); Mague *et al.* (2007). For details of the Cambridge Crystallographic Database, see: Allen (2002).



Experimental

Crystal data

$C_{17}H_{19}O_2PSe$
M_r = 365.25
Monoclinic, $P2_1/c$
a = 9.6212 (5) Å
b = 10.3914 (5) Å
c = 17.1087 (9) Å
β = 99.618 (5)°
V = 1686.45 (15) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.32 mm^{-1}
T = 120 K
0.22 × 0.2 × 0.12 mm

Data collection

Oxford Diffraction KM-4-CCD diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2008)
T_{min} = 0.588, T_{max} = 0.760
12450 measured reflections
3674 independent reflections
2596 reflections with $I > 2\sigma(I)$
R_{int} = 0.06

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.147
S = 0.97
3674 reflections
193 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 2.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.65 e Å^{-3}

Table 1
Comparison of the geometry of the title compound with related compounds (Å, °).

CSD refcode (Allen, 2002)	P—Se	P—O	Ph–Ph dihedral	Smaller torsion	Reference
	2.0769 (11)	1.650 (3)	72.64 (14)	7.0 (4)	This work
MPSEPO	2.080	1.619	82.62	4.15	Lepicard *et al.* (1969)
MUMFUV	2.072	1.624	80.93	13.32	Balakrishna *et al.* (2002)
	2.070	1.612	75.01	22.34	
RAMXEJ	2.089	1.596	78.65	8.84	Balakrishna *et al.* (2005)
	2.079	1.585	78.49	6.58	
YIQOM	2.089	1.620	70.15	6.15	Mague *et al.* (2007)

Data collection: *CrysAlis CCD* (Oxford Diffraction 2008); cell refinement: *CrysAlis RED* (Oxford Diffraction 2008); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: EZ2163).

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