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O-4-Chlorobenzoyl diphenylselenophosphinate

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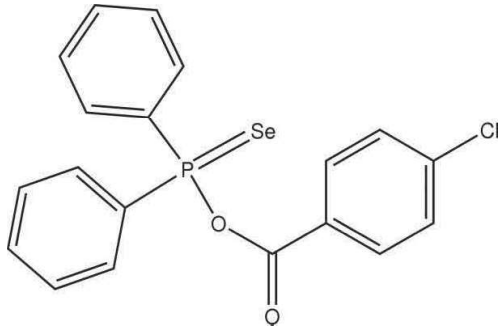
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.006 Å; R factor = 0.054; wR factor = 0.162; data-to-parameter ratio = 19.2.

The title compound, $C_{19}H_{14}ClO_2PSe$, was obtained in the reaction of the diphenylmonoselenophosphinic acid ammonium salt with 4-chlorobenzoyl chloride. The dihedral angle between the P-bonded aromatic rings is 72.64 (14)°. Packing of the molecules in the crystal is reinforced by π–π stacking interactions between two inversion-related 4-chlorobenzene rings [centroid-centroid separation = 4.189 (2) Å] and a C—H···O interaction also occurs.

Related literature

Syntheses of *O*-acyl monoselenophosphates have already been described by Rachon *et al.* (2005); Mielniczak & Łopusinski (2001). For a related *O*-acyl derivative, see Cholewinski *et al.* (2009). For related *O*-alkyl or *O*-aryl derivatives, see: Lepicard *et al.* (1969); Balakrishna *et al.* (2002, 2005); Mague *et al.* (2007).



Experimental

Crystal data

$C_{19}H_{14}ClO_2PSe$ M_r = 419.68
Monoclinic, $P2_1/c$
a = 9.3390 (5) Å
b = 9.7132 (5) Å
c = 19.1353 (15) Å
β = 97.059 (6)°
V = 1722.64 (19) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.44 mm^{-1}
T = 120 K
0.46 × 0.33 × 0.26 mm

Data collection

Oxford Diffraction KM-4-CCD diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2008)
T_{min} = 0.325, T_{max} = 0.53
14128 measured reflections
4158 independent reflections
3376 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.162
S = 1.16
4158 reflections
217 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.82 e Å^{-3}
$\Delta\rho_{min}$ = −0.56 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C16—H16···O2^{i}	0.95	2.59	3.359 (6)	138

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

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: EZ2164).

References

Balakrishna, M. S., George, P. P. & Mobin, S. M. (2005). *Polyhedron*, **24**, 475–480.
Balakrishna, M. S., Panda, R. & Mague, J. T. (2002). *J. Chem. Soc. Dalton Trans.* pp. 4617–4621.
Cholewinski, G., Chojnacki, J., Pikies, J. & Rachon, J. (2009). *Acta Cryst.* E**65**, o853–o854.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Lepicard, G., de Saint-Giniez-Liebig, D., Laurent, A. & Rérat, C. (1969). *Acta Cryst.* B**25**, 617–624.
Mague, J. T., Punji, B., Ganesamoorthy, C. & Balakrishna, M. S. (2007). *Acta Cryst.* E**63**, o4645.
Mielniczak, G. & Łopusinski, A. (2001). *Synth. Commun.* **31**, 3659–3664.
Oxford Diffraction (2008). *CrysAlis CCD* and *CrysAlis RED*. Oxford Diffraction Ltd, Abingdon, England.
Rachon, J., Cholewinski, G. & Witt, D. (2005). *Chem. Commun.* pp. 2692–2694.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.