Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

5,5-Dimethyl-2-methylseleno-1,3,2-dioxaphosphorinan-2-one

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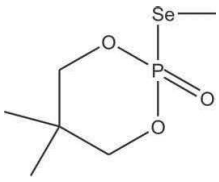
Received 27 February 2010; accepted 4 March 2010

Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.005 Å; R factor = 0.026; wR factor = 0.065; data-to-parameter ratio = 12.0.

The title compound, $C_6H_{13}O_3PSe$, was obtained in the reaction of 5,5-dimethyl-2-oxo-2-seleno-1,3,2-dioxaphosphorinane potassium salt with methyl iodide. The selenomethyl group is in the axial position in relation to the six-membered dioxaphosphorinane ring.

Related literature

For the structures of similar methyl esters with >P(Se)OMe and >P(Se)SeMe groups, see: Grand *et al.* (1975); Bartczak *et al.* (1987). For 5,5-dimethyl-2-seleno-1,3,2-dioxaphosphorinane derivatives with equatorial Se atoms, see: Bartczak & Wolf (1983); Bartczak *et al.* (1983); Wolf & Bartczak (1989) and for *O*-acyl derivatives with equatorial selenium, see: Cholewinski *et al.* (2009). For conformers with axial Se atoms, see: Bartczak *et al.* (1986); Potrzebowski *et al.* (1994); Wieczorek *et al.* (1995). For details of the synthesis, see: Rachon *et al.* (2005); Stec (1974). For a description of the Cambridge Structural Database, see: Allen (2002).



Experimental

Crystal data

$C_6H_{13}O_3PSe$
M_r = 243.09
Monoclinic, *Cc*
a = 9.2252 (4) Å
b = 9.4842 (4) Å
c = 11.4160 (6) Å
β = 101.078 (5)°
V = 980.22 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.96 mm^{-1}
T = 150 K
0.59 × 0.41 × 0.28 mm

Data collection

Oxford Diffraction KM-4-CCD diffractometer
Absorption correction: analytical [*CrysAlis RED* (Oxford Diffraction, 2009), using a multi-faceted crystal model based on expressions derived by Clark & Reid (1995)]
T_{min} = 0.179, T_{max} = 0.372
3146 measured reflections
1238 independent reflections
1214 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.065
S = 1.05
1238 reflections
103 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.69 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}
Absolute structure: Flack (1983), 189 Friedel pairs
Flack parameter: −0.009 (10)

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2009); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2009); 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) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *WinGX* (Farrugia, 1999), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2544).

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