Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Isopropyl 2-(5,7-dimethyl-1,2,4-triazolo[1,5-*a*]-pyrimidin-2-yloxy)benzoate

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Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.004 Å
R factor = 0.059
wR factor = 0.159
Data-to-parameter ratio = 14.7

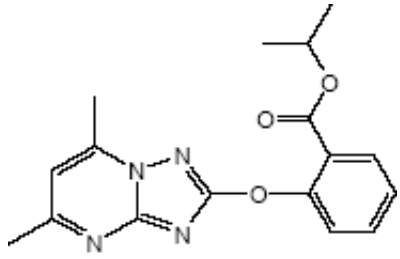
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 31 May 2005
Accepted 6 June 2005
Online 17 June 2005

In the title compound, $C_{17}H_{18}N_4O_3$, which displays good herbicidal activity, the planar bicyclic triazolopyrimidine system is bound to the benzoic acid isopropyl ester moiety *via* an O bridge. The dihedral angle formed by the bicylic triazolopyrimidine system and the benzene ring is 106.2 (2)°. Neither intra- nor intermolecular hydrogen bonds are found.

Comment

Triazolopyrimidine compounds exhibit a wide spectrum of biological activity; many have been developed as effective herbicides, and others have been used as therapeutic agents. The title compound, (I), may be used as a new precursor for obtaining bioactive molecules. In this paper, we present the X-ray crystallographic analysis of (I).



(I)

The molecular structure of (I) is shown in Fig. 1. The triazolopyrimidine ring system is planar to within 0.03 Å. It is bound to the benzoic acid isopropyl ester moiety *via* an O bridge. The dihedral angle formed by the mean planes of the

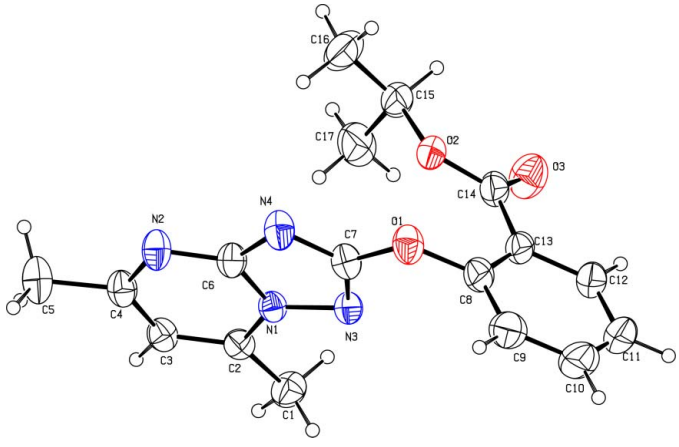


Figure 1
A view of the molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are represented by circles of arbitrary size.

triazolopyrimidine and benzene ring systems (C7/N3/N1/C2–C4/N2/C6/N4 and C8–C13) is 106.2 (2)°.

Experimental

A mixture of 2-hydroxybenzoic acid isopropyl ester (4 mmol) and sodium hydride (4 mmol) in anhydrous toluene (60 ml) was stirred at 373 K for 2 h. 2-Methylsulfonyl-1,2,4-triazolo[1,5-*a*]pyrimidine (1 mmol) was then added and the resulting reaction mixture refluxed for about 20 h. After filtration, the solvent was removed under reduced pressure and the residue was purified by column chromatography on silica gel, with petroleum ether–acetone (4:1 *v*/*v*) as eluent, to afford the title compound, (I) (yield 40%, m.p. 395 K). Crystals suitable for single-crystal X-ray diffraction were grown from acetone at 277 K. Spectroscopic analysis: ^{1}H NMR ($CDCl_3$, 400 MHz, δ, p.p.m.): 7.33–8.04 (*m*, 4H, Ar—H), 6.75 (*s*, 1H, 6H),5.09 (*m*, 1H, CH), 2.71 (*s*, 3H, 7CH_3), 2.59 (*s*, 3H, 5CH_3), 1.16 (*d*, 6H, CH_3); MS (EI, 70 eV), *m*/*z* (%): 326 (9), 267 (24), 239 (100), 196 (10), 92 (12), 67 (12).

Crystal data

$C_{17}H_{18}N_4O_3$
M_r = 326.35
Monoclinic, $P2_1/c$
a = 15.1169 (18) Å
b = 10.7393 (13) Å
c = 10.2017 (13) Å
β = 95.839 (3)°
V = 1647.6 (3) Å^3
Z = 4
D_x = 1.316 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1157 reflections
θ = 2.7–19.8°
μ = 0.09 mm^{-1}
T = 292 (2) K
Block, colourless
0.20 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1996)
T_{min} = 0.982, T_{max} = 0.991
8828 measured reflections
3238 independent reflections
1950 reflections with $I > 2\sigma(I)$
R_{int} = 0.053
θ_{max} = 26.0°
$h = -18 \rightarrow 9$
$k = -13 \rightarrow 12$
$l = -11 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.159
S = 1.03
3238 reflections
221 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0684P)^2 + 0.0513P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

H atoms were placed in calculated positions and treated as riding atoms, with C—H = 0.93 and 0.96 Å and with U_{iso}(H) = 1.2U_{eq}(CH) or 1.5U_{eq}(CH_3).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

The authors acknowledge financial support from the National Key Project for Basic Research (grant No. 2002CCA00500), the National Natural Science Foundation of China (grant Nos. 20432010, 20476036 and 20172017), the Programme for New Century Excellent Talents in Universities of China and the Programme for Excellent Research Groups of Hubei Province (grant No. 2004ABC002).

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