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(*E*)-3-(4-Fluorophenyl)-1-(2-nitrophenyl)prop-2-en-1-one

Zhi-fang Pan

Microscale Science Institute, Weifang University, Weifang 261061, People's Republic of China
Correspondence e-mail: weichidu@163.com

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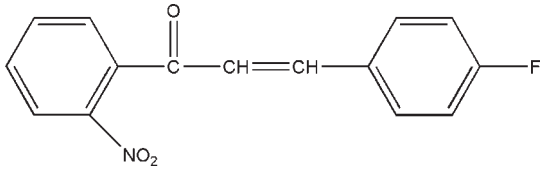
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.044; wR factor = 0.141; data-to-parameter ratio = 16.1.

The title compound, $C_{15}H_{10}F_NO_3$, was prepared from 2-nitroacetphenone and 4-fluorobenzaldehyde by an Aldol condensation reaction. The dihedral angle formed by the two benzene rings is 67.37 (2)°. The crystal structure is stabilized by weak intermolecular C—H···O and C—H···F hydrogen bonds.

Related literature

For the biological activities of chalcones, see: Hsieh *et al.* (1998); Anto *et al.* (1994); De Vincenzo *et al.*(2000); Dimmock *et al.* (1998). For related structures, see: Fun *et al.* (2008); Guo *et al.* (2009).



Experimental

Crystal data

$C_{15}H_{10}FNO_3$
M_r = 271.24
Monoclinic, $P2_1/n$
a = 7.7698 (16) Å
b = 17.072 (3) Å
c = 9.759 (2) Å
β = 96.72 (3)°
V = 1285.6 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 293 K
0.3 × 0.3 × 0.2 mm

Data collection

Bruker SMART CCD diffractometer
12293 measured reflections
2921 independent reflections
2218 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.141
S = 1.13
2921 reflections
181 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4A···O3^{i}	0.93	2.57	3.500 (2)	177
C5—H5A···F1^{ii}	0.93	2.54	3.396 (2)	153
C9—H9A···O3^{iii}	0.93	2.57	3.411 (2)	150

Symmetry codes: (i) $x+1, y, z$; (ii) $-x+1, -y, -z+2$; (iii) $-x, -y, -z+1$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5041).

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