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trans-3-(3,4-Dimethoxyphenyl)-2-(4-nitrophenyl)prop-2-enenitrile

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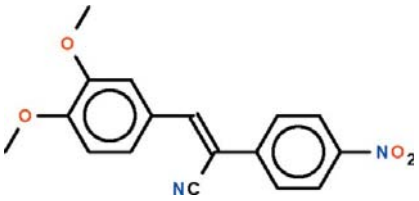
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.047; wR factor = 0.133; data-to-parameter ratio = 16.0.

The asymmetric unit of the title compound, $C_{17}H_{14}N_2O_4$, contains two independent molecules in which the benzene rings are in a *trans* arrangement with respect to the C=C double bond and the rings are inclined by 4.3 (1) and 22.1 (1)° with respect to each other.

Related literature

For the crystal structure of α-((4-methoxyphenyl)methylene)-4-nitrobenzeneacetonitrile, see: Vrcelj *et al.* (2002). For background literature on this class of pigments, see: Asiri (1999).



Experimental

Crystal data

$C_{17}H_{14}N_2O_4$
M_r = 310.30
Triclinic, $P\overline{1}$
a = 10.2211 (8) Å
b = 11.9460 (9) Å
c = 12.2764 (10) Å
α = 91.094 (1)°
β = 99.542 (1)°
γ = 100.156 (1)°
V = 1453.3 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 100 K
0.40 × 0.20 × 0.10 mm

Data collection

Bruker SMART APEX diffractometer
13853 measured reflections
6628 independent reflections
4851 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.133
S = 1.02
6628 reflections
415 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5073).

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