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2-Benzylmalononitrile

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Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.003 Å
R factor = 0.055
wR factor = 0.174
Data-to-parameter ratio = 17.8

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

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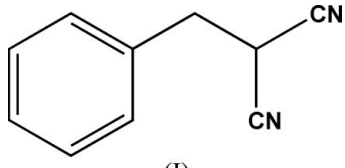
The reaction of 5-methyl-2-phenyl-2*H*-1,2,4-triazol-3(4*H*)-one, benzaldehyde and malononitrile in ethanol in the presence of triethylamine produced the title compound, $C_{10}H_8N_2$, rather than the anticipated polysubstituted 2,6-dicyanoaniline. The plane defined by the phenyl *ipso*-C atom, the methylene C atom and the central C atom of the malononitrile group is roughly orthogonal to the benzene ring plane [dihedral angle = 81.6 (2)°]; one of the nitrile groups of the malononitrile almost lies in this plane [corresponding C(Ph)—CH_2—C—CN torsion angle = 176.06 (17)°].

Comment

Cui *et al.* (2005) synthesized polysubstituted 2,6-dicyanoanilines *via* a three-component reaction of aldehydes, ketones and malononitrile in the presence of triethylamine. We attempted to conduct this reaction using 5-methyl-2-phenyl-2*H*-1,2,4-triazol-3(4*H*)-one as a ketone component. However, we were unable to find any of the expected polysubstituted 2,6-dicyanoanilines among the products of this reaction. Instead. we isolated the title compound, 2-benzylmalononitrile, (I).



(I)

The plane of the benzene ring C1–C6 (plane *A*) is roughly orthogonal to the plane defined by atoms C6, C7 and C8 (plane *B*); the dihedral angle *A*/*B* is 81.6 (2)°. One of the nitrile groups (C9 ≡N1) lies almost exactly in plane *B*, the C6—C7—C8—C9 torsion angle being 176.06 (17)°.

Experimental

5-Methyl-2-phenyl-2*H*-1,2,4-triazol-3(4*H*)-one (0.175 g, 1 mmol) and malononitrile (0.183 g, 2.5 mmol) were added with stirring to a solution of benzaldehyde (0.106 g, 1 mmol) in EtOH (8 ml) in the presence of triethylamine (0.151 g, 1.5 mmol). The reaction mixture was then refluxed for 10 h and monitored by thin-layer chromatography. Upon completion of the reaction, the solvent was evaporated *in vacuo* and the residue was purified by chromatography on silica using a petroleum ether/diethyl ether (10:1) mixture as eluent to give 2-benzylmalononitrile [yield 15%; m.p. 359–361 K, literature m.p. 362–363 K (Diez-Barra *et al.*, 1991)]. Crystals suitable for X-ray diffraction analysis were grown from ethanol.

Crystal data

$C_{10}H_8N_2$
$M_r = 156.18$
Monoclinic, $P2_1/c$
$a = 5.8391\ (13)$ Å
$b = 15.145\ (4)$ Å
$c = 9.807\ (2)$ Å
$\beta = 99.270\ (5)^\circ$
$V = 856.0\ (3)$ Å^3
$Z = 4$
$D_x = 1.212$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.07$ mm^{-1}
$T = 292\ (2)$ K
Block, colourless
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.978$, $T_{max} = 0.985$
6068 measured reflections
1942 independent reflections
1061 reflections with $I > 2\sigma(I)$
$R_{int} = 0.099$
$\theta_{max} = 27.5^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.174$
$S = 0.94$
1942 reflections
109 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0839P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-3}

All H atoms were initially located in a difference Fourier map, then placed in idealized positions (C—H = 0.93 Å for aromatic and 0.97 Å for aliphatic H atoms) and included in the refinement using a riding-model approximation, with $U_{iso}(H) = 1.2U_{eq}(C)$.

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*.

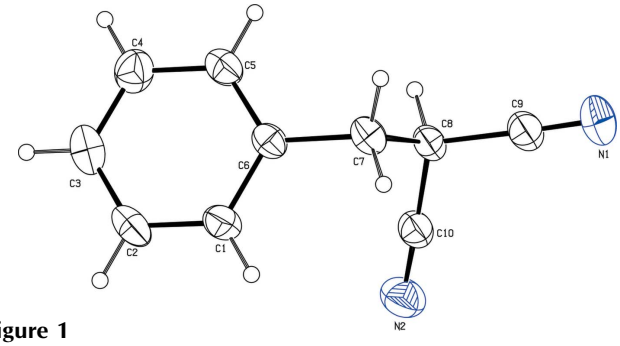


Figure 1
The molecular structure of (I), showing the atom-labelling scheme and displacement ellipsoids drawn at the 50% probability level.

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