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Key indicators

Single-crystal X-ray study

T = 296 K

Mean σ(C-C) = 0.004 Å

R = 0.060

wR = 0.165

Data-to-parameter ratio = 17.2

Details

(*E*)-2-Cyano-3-[4-(dimethylamino)phenyl]-*N*-phenylprop-2-enamide

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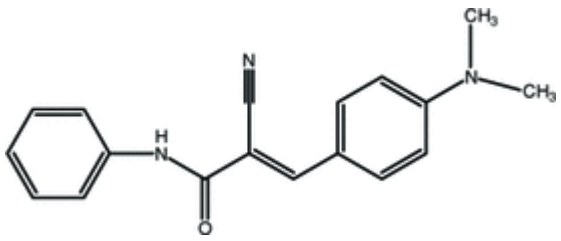
In the title compound, $C_{18}H_{17}N_3O$, the dihedral angle between the phenyl and benzene rings is 11.22 (14)°. Apart from the methyl H atoms, the molecule is close to planar, with a maximum deviation of 0.145 (3) Å. Intramolecular C-H...O and C-H...N interactions occur. In the crystal, inversion dimers linked by pairs of N-H...N hydrogen bonds occur, resulting in an $R_2^2(12)$ ring motif. Further C-H...N and C-H...O bonds generate $R_1^2(7)$ and $R_2^2(22)$ motifs and a C-H...π interaction also occurs.

Related literature

For background on the properties and uses of organic dyes, see: Grabowski *et al.* (2003); Guo *et al.* (2007); Kwak *et al.* (2008); Moylan *et al.* (1996). For reference structural data, see Allen *et al.* (1987). For graph-set terminology, see: Bernstein *et al.* (1995).



Experimental

Crystal data

- $C_{18}H_{17}N_3O$
- M_r = 291.35
- Monoclinic, $P\,2_1/c$

- a = 12.0639 (19) Å
- b = 19.983 (3) Å
- c = 6.3960 (9) Å
- β = 94.870 (6)°
- V = 1536.3 (4) Å^3
- Z = 4
- Mo $K\alpha$ radiation
- μ = 0.08 mm^{-1}
- T = 296 K
- 0.44 × 0.09 × 0.07 mm

Data collection

- Bruker Kappa APEXII CCD diffractometer
- Absorption correction: none
- 15701 measured reflections
- 3484 independent reflections
- 1380 reflections with $I > 2\sigma(I)$
- R_{int} = 0.082

Refinement

- $R[F^2 > 2\sigma(F^2)]$ = 0.060
- $wR(F^2)$ = 0.165
- S = 0.97
- 3484 reflections
- 202 parameters
- H-atom parameters constrained
- $\Delta\rho_{max}$ = 0.19 e Å^{-3}
- $\Delta\rho_{min}$ = -0.16 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °)

D-H···*A*	*D*-H	H···*A*	*D*···*A*	*D*-H···*A*
C5-H5···O1	0.93	2.30	2.892 (4)	121
C12-H12···N2	0.93	2.61	3.445 (4)	149
N1-H1*A*···N2^{i}	0.86	2.50	3.245 (3)	146
C1-H1···N2^{i}	0.93	2.58	3.338 (4)	139
C18-H18*A*···O1^{ii}	0.96	2.49	3.439 (4)	169
C3-H3···*Cg*1^{iii}	0.93	2.66	3.514 (3)	152

Symmetry codes: (i) -*x*, -*y*, -*z*+1; (ii) -*x*+1, -*y*, -*z*; (iii) $x, -y+\frac{1}{2}, z+\frac{1}{2}$. *Cg*1 is the centroid of the C1-C6 phenyl ring.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SIR97* (Altomare *et al.*,

1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2974).

Acknowledgements

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References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1-19.
Altomare, A., Burla, M. C., Camalli, M., Cascarano, G. L., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). *J. Appl. Cryst.* **32**, 115-119. CrossRef ChemPort details
Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555-1573. CrossRef ChemPort
Bruker (2007). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565. CrossRef details
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837-838. CrossRef details
Grabowski, Z. R., Rotkiewicz, K. & Rettig, W. (2003). *Chem. Rev.* **103**, 3899-4031. CrossRef PubMed
Guo, Z. Q., Zhu, W. H., Shen, L. J. & Tian, H. (2007). *Angew. Chem. Int. Ed.* **46**, 5549-5553. CrossRef ChemPort
Kwak, G., Wang, S., Choi, M. S., Kim, H., Choi, K. H., Han, Y. S., Hur, Y. & Kim, S. H. (2008). *Dyes Pigments*, **78**, 25-33. CrossRef ChemPort
Moylan, C. R., Ermer, S., Lovejoy, S. M., McComb, I. H., Leung, D. S., Wortmann, R., Krdmer, P. & Twieg, R. J. (1996). *J. Am. Chem. Soc.* **118**, 12950-12955. CrossRef ChemPort
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112-122. CrossRef details
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148-155. CrossRef details

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