

2,3-Dimethyl-N-[(*E*)-2,4,5-trimethoxybenzylidene]aniline

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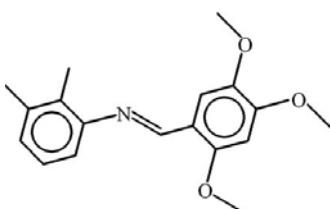
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Key indicators: single-crystal X-ray study; $T = 296\text{ K}$; mean $\sigma(\text{C}-\text{C}) = 0.002\text{ \AA}$; R factor = 0.045; wR factor = 0.139; data-to-parameter ratio = 19.4.

In the title compound, $\text{C}_{18}\text{H}_{21}\text{NO}_3$, the $\text{C}=\text{N}$ bond has a *trans* conformation and the benzene rings are oriented at a dihedral angle of $61.32(6)^\circ$. The C atoms of the three methoxy groups are all roughly coplanar with their attached ring [deviations = $0.219(2)$, $-0.097(2)$ and $-0.137(2)\text{ \AA}$]. In the crystal, a weak $\text{C}-\text{H}\cdots\pi$ interaction may help to establish the packing.

Related literature

For background information on Schiff bases and related crystal structures, see: Tahir *et al.* (2010a,b); Tariq *et al.* (2010).



Experimental

Crystal data

$\text{C}_{18}\text{H}_{21}\text{NO}_3$
 $M_r = 299.36$
Triclinic, $P\bar{1}$
 $a = 7.0040(2)\text{ \AA}$
 $b = 11.0396(4)\text{ \AA}$

$c = 11.1585(4)\text{ \AA}$
 $\alpha = 73.941(1)^\circ$
 $\beta = 76.022(2)^\circ$
 $\gamma = 82.079(1)^\circ$
 $V = 802.24(5)\text{ \AA}^3$

$Z = 2$
Mo $K\alpha$ radiation
 $\mu = 0.08\text{ mm}^{-1}$

$T = 296\text{ K}$
 $0.32 \times 0.14 \times 0.12\text{ mm}$

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
 $T_{\min} = 0.980$, $T_{\max} = 0.985$

13855 measured reflections
3957 independent reflections
2935 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.024$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.045$
 $wR(F^2) = 0.139$
 $S = 1.07$
3957 reflections

204 parameters
H-atom parameters constrained
 $\Delta\rho_{\max} = 0.23\text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.16\text{ e \AA}^{-3}$

Table 1

Hydrogen-bond geometry (\AA , $^\circ$).

$Cg1$ is the centroid of the C1–C6 ring.

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{Cl}6-\text{H}16B\cdots Cg1^i$	0.96	2.99	3.5694 (19)	120

Symmetry code: (i) $-x + 2$, $-y + 1$, $-z + 1$.

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: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5535).

References

- Bruker (2005). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Bruker (2009). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
- Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
- Sheldrick, G. M. (2008). *Acta Cryst. A* **64**, 112–122.
- Spek, A. L. (2009). *Acta Cryst. D* **65**, 148–155.
- Tahir, M. N., Tariq, M. I., Ahmad, S., Sarfraz, M. & Ather, A. Q. (2010a). *Acta Cryst. E* **66**, o1562.
- Tahir, M. N., Tariq, M. I., Ahmad, S., Sarfraz, M. & Ather, A. Q. (2010b). *Acta Cryst. E* **66**, o1817.
- Tariq, M. I., Ahmad, S., Tahir, M. N., Sarfraz, M. & Hussain, I. (2010). *Acta Cryst. E* **66**, o1561.