4-(3,4-Dimethyl-5-phenyl-1,3-oxazolidin-2-yl)-2-methoxyphenol

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Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.004 Å; R factor = 0.043; wR factor = 0.096; data-to-parameter ratio = 10.3.

In the title compound, C18H21NO3, the oxazolidine ring adopts an envelope conformation with the N atom at the flap position. The two benzene rings make dihedral angles of 74.27 (14) and 73.26 (15)° with the mean plane through the oxazolidine ring. In the crystal structure, O—H···O and C—H···O hydrogen bonds connect adjacent molecules into chains along [010] incorporating R2(8) loops and further stabilization is provided by weak intermolecular C—H···π interactions.

Related literature

For general background to and applications of the title oxazolidine compound, see: Fitzgerald et al. (2005); Kamat et al. (2000); Kumar et al. (2004); Walton et al. (2003). For graph-set descriptions of hydrogen-bond ring motifs, see: Bernstein et al. (1995). For a related structure, see: Duffy et al. (2004). For bond-length data, see: Allen et al. (1987). For the stability of the temperature controller used for the data collection, see: Cosier & Glazer (1986).

Experimental

Crystal data

C18H21NO3

| Parameter         | Value          |
|-------------------|----------------|
| M_r             | 299.36         |
| orthorhombic     | P212121        |
| a = 11.7697 (9) Å |                |
| b = 11.2697 (9) Å |                |
| c = 17.4392 (13) Å |               |
| V = 1619.3 (2) Å³ |                |
| Z                  | 4              |
| Mo Kα radiation  |                |
| μ = 0.08 mm⁻¹ |                |
| T = 120 K         |                |
| 9140 measured reflections | 1622 reflections with I > 2σ(I) |
| H atoms treated by a mixture of independent and constrained refinement | Δρ_max = 0.19 e Å⁻³ |
| Δρ_min = −0.21 e Å⁻³ |

Data collection

Bruker SMART APEXII CCD diffractometer

Absorption correction: multi-scan (SADABS; Bruker, 2009)

2131 independent reflections

206 parameters

Refinement

R[F² > 2σ(F²)] = 0.043

wR(F²) = 0.096

Symmetry codes:

(i) −x + 1, y − 1/2, −z + 1/2
(ii) −x + 1, y + 1/2, −z + 1/2
(iii) −x, −y, −z

Table 1

Hydrogen-bond geometry (Å, °).

Cg1 is the centroid of the C10-C15 phenyl ring.

Data collection: APEX2 (Bruker, 2009); cell refinement: SAINT (Bruker, 2009); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL and PLATON (Spek, 2009).

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