

2-Phenylimidazo[1,2-a]pyridine-3-carbaldehyde

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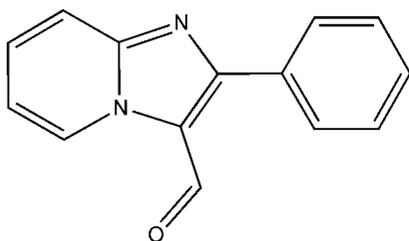
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Key indicators: single-crystal X-ray study; $T = 120$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.032; wR factor = 0.078; data-to-parameter ratio = 14.3.

In the title compound, $\text{C}_{14}\text{H}_{10}\text{N}_2\text{O}$, the dihedral angle between the imidazo[1,2-*a*]pyridine and phenyl rings is $28.61(4)^\circ$. The molecules are connected into broad chains parallel to the *a* axis by weak $\text{C}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{N}$ hydrogen bonds. The linking of the ribbons is provided by $\pi-\pi$ stacking interactions between neighbouring pyridine rings, with a centroid-centroid distance of $3.7187(7)$ Å.

Related literature

For general background, see Anafloous *et al.* (2008) and references therein. For related literature, see: Meth-Cohn & Stanforth (1991).



Experimental

Crystal data

$\text{C}_{14}\text{H}_{10}\text{N}_2\text{O}$
 $M_r = 222.2$
Orthorhombic, $Pbca$
 $a = 13.0640(3)$ Å
 $b = 7.4162(2)$ Å
 $c = 21.6698(6)$ Å
 $V = 2099.48(9)$ Å³
 $Z = 8$
Mo $K\alpha$ radiation
 $\mu = 0.09$ mm⁻¹
 $T = 120$ K
 $0.57 \times 0.40 \times 0.24$ mm

Data collection

Oxford Diffraction Xcalibur2 diffractometer with Sapphire2 CCD detector
Absorption correction: none
25795 measured reflections
2196 independent reflections
1305 reflections with $I > 3\sigma(I)$
 $R_{\text{int}} = 0.049$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.031$
 $wR(F^2) = 0.077$
 $S = 1.04$
2196 reflections
154 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.15$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.16$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-\text{H}\cdots A$ | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|--|--------------|--------------------|-------------|----------------------|
| $\text{C4}-\text{H4}\cdots\text{N1}^{\text{i}}$ | 0.96 | 2.50 | 3.4386 (18) | 165 |
| $\text{C6}-\text{H6}\cdots\text{O1}^{\text{ii}}$ | 0.96 | 2.46 | 3.1856 (16) | 133 |

Symmetry codes: (i) $-x + 1, -y, -z$; (ii) $-x, -y, -z$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SIR2002* (Burla *et al.*, 2003); program(s) used to refine structure: *JANA2000* (Petříček *et al.*, 2000); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2005); software used to prepare material for publication: *JANA2000*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2180).

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