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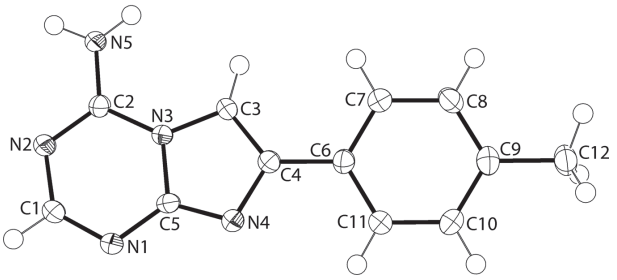
# Crystal structure of 7-(4-methylphenyl)imidazo [1,2-*a*][1, 3, 5]triazin-4-amine, $C_{12}H_{11}N_5$

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**Abstract**

$C_{12}H_{11}N_5$, monoclinic, $P2_1/n$ (no. 14), $a = 7.3455(1)$ Å, $b = 12.2470(1)$ Å, $c = 12.1689(1)$ Å, $\beta = 103.505(1)°$, $V = 1064.45(2)$ Å$^3$, $Z = 4$, $R_{gt}(F) = 0.0365$, $wR_{ref}(F^2) = 0.0987$, $T = 100$ K.

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The asymmetric unit of the title crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

## Source of material

The compound was prepared and characterised as described in the literature [5]. Crystals for the crystallographic study were obtained from the slow evaporation of a very dilute methanol solution.

## Experimental details

The C-bound H atoms were geometrically placed (C—H = 0.98−0.99 Å) and refined as riding with $U_{iso}(H) = 1.2$–$1.5U_{eq}(C)$. The N-bound hydrogen atoms were located in difference Fourier maps, but were refined with a distance restraint of N—H = 0.88 ± 0.01 Å, and with unconstrained $U_{iso}(H)$.

**Table 1:** Data collection and handling.

| | |
|---|---|
| Crystal: | Block, colourless |
| Size: | 0.44 × 0.16 × 0.09 mm |
| Wavelength: | Cu $K\alpha$ radiation (1.54184 Å) |
| $\mu$: | 0.73 mm$^{-1}$ |
| Diffractometer, scan mode: | SuperNova, $\varphi$ and $\omega$-scans |
| $\theta_{max}$, completeness: | 76.5°, >99% |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$, $R_{int}$: | 18249, 2225, 0.026 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\,\sigma(I_{obs})$, 2132 |
| $N(param)_{refined}$: | 163 |
| Programs: | CrysAlis$^{PRO}$ [1], SHELX [2, 3], WinGX and ORTEP [4] |

## Discussion

The 5-aza-7-deaza-isostere (imidazo[1,2-a][1, 3, 5]triazine) of the purine system is an important scaffold for the construction of various drugs. Such compounds have been developed as inhibitors for enzymes, e.g. focal adhesion kinase [6]. Further, these compounds display anti-viral activity [7], are agonists of opioid m-receptors [8] and function as ligands for adenosine receptors [9]. A hindrance to the embellishment of this class of compound has been the difficulty in their synthesis. Very recently, a new procedure for the synthesis of 5-aza-7-deaza-isosteres was developed, i.e. through the reaction of 2-aminoimidazoles, triethylorthoformate and cyanamide under microwave irradiation [5]. The title compound was one of the new compounds synthesised in the course of that study.

The title molecule is shown in the figure (70% displacement ellipsoids) and comprises a six- and five-membered fused ring system connected to the 4-methylphenyl group at C4. The r.m.s. deviation of the nine atoms of the imidazotriazine group is 0.0218 Å with the maximum deviations being 0.0399(7) Å for the C2 atom and to the other side of the least-squares plane, 0.0273(7) Å for the C3 atom. The amino-N5 atom lies 0.1258(13) Å out of the plane in the direction of the C2 atom. There is a twist between this plane and that through the appended 4-methylphenyl group as seen in the dihedral angle of 12.39(4)° formed between them. The overall molecular geometry resembles that reported for the 4-methoxyphenyl derivative [5].

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**Table 2:** Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$).

| Atom | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| N1 | 0.65755(12) | 0.76747(7) | 0.76013(7) | 0.0160(2) |
| N2 | 0.56271(12) | 0.90789(7) | 0.62085(7) | 0.0152(2) |
| N3 | 0.43165(12) | 0.73441(7) | 0.58693(7) | 0.0135(2) |
| N4 | 0.51177(12) | 0.59379(7) | 0.70583(7) | 0.0153(2) |
| N5 | 0.35748(13) | 0.86947(7) | 0.44944(7) | 0.0167(2) |
| H1N | 0.2954(19) | 0.8213(10) | 0.4000(11) | 0.027(4)* |
| H2N | 0.382(2) | 0.9366(8) | 0.4286(12) | 0.026(4)* |
| C1 | 0.65857(14) | 0.86774(8) | 0.72106(8) | 0.0158(2) |
| H1 | 0.7367 | 0.9183 | 0.7696 | 0.019* |
| C2 | 0.45045(14) | 0.83930(8) | 0.55095(8) | 0.0137(2) |
| C3 | 0.32629(14) | 0.64623(8) | 0.53665(8) | 0.0145(2) |
| H3 | 0.2379 | 0.6448 | 0.4659 | 0.017* |
| C4 | 0.37712(14) | 0.56166(8) | 0.61100(8) | 0.0143(2) |
| C5 | 0.54085(14) | 0.69780(8) | 0.68995(8) | 0.0139(2) |
| C6 | 0.30889(14) | 0.44836(8) | 0.59856(8) | 0.0147(2) |
| C7 | 0.20768(15) | 0.40938(9) | 0.49422(9) | 0.0175(2) |
| H7 | 0.1760 | 0.4576 | 0.4315 | 0.021* |
| C8 | 0.15305(15) | 0.30053(9) | 0.48163(9) | 0.0184(2) |
| H8 | 0.0847 | 0.2754 | 0.4100 | 0.022* |
| C9 | 0.19638(14) | 0.22754(8) | 0.57174(9) | 0.0172(2) |
| C10 | 0.29339(15) | 0.26757(8) | 0.67647(9) | 0.0186(2) |
| H10 | 0.3222 | 0.2196 | 0.7395 | 0.022* |
| C11 | 0.34874(15) | 0.37631(8) | 0.69031(9) | 0.0172(2) |
| H11 | 0.4140 | 0.4018 | 0.7625 | 0.021* |
| C12 | 0.14124(16) | 0.10914(9) | 0.55662(9) | 0.0212(2) |
| H12A | 0.0357 | 0.0951 | 0.5912 | 0.032* |
| H12B | 0.2476 | 0.0633 | 0.5930 | 0.032* |
| H12C | 0.1045 | 0.0919 | 0.4758 | 0.032* |

As anticipated, the molecular packing features a number of conventional hydrogen-bonding interactions. Thus, centrosymmetricaly related molecules associate *via* amine-N—H$\cdots$N(triazine) hydrogen bonds and eight-membered $\{\cdots HNCN\}_2$ synthons [N5—H2n$\cdots$N2: 2.066(11) Å and 179.6(17)° for symmetry operation $1-x, 2-y, 1-z$]. The dimeric aggregates are connected into twisted, one-dimensional supramolecular chains, parallel to [1 0 $\bar{1}$], *via* amine-H$\cdots$amine-N—H$\cdots$N(triazine) hydrogen bonds, involving the other amine-H and triazine-N atoms [N5—H1n$\cdots$N1: 2.074(13) Å and 168.2(12)° for symmetry operation $-1/2+x$, $3/2-y$, $-1/2+z$].

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