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N-(4-Amino-2-methoxyphenyl)acetamide

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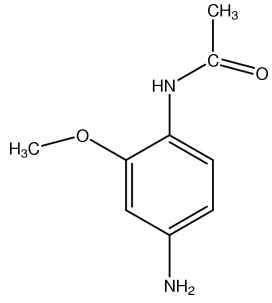
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.063
wR factor = 0.225
Data-to-parameter ratio = 14.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $C_9H_{12}N_2O_2$, is the product of the second step in the synthesis of *N*-(4-amino-3-methoxyphenyl)-methanesulfonamide, the side chain of an anticancer drug (*viz.* Amsacrine). The compound, obtained by the reduction of *N*-(2-methoxy-4-nitrophenyl)acetamide in EtOH with Pd/C as catalyst, under a hydrogen atmosphere, crystallizes from ethylacetoacetate.



(I)

Experimental

The title compound was obtained by the reduction of *N*-(2-methoxy-4-nitrophenyl)acetamide in EtOH with Pd/C as catalyst, under a hydrogen atmosphere, and was crystallized from ethylacetoacetate.

Crystal data

$C_9H_{12}N_2O_2$
M_r = 180.21
Orthorhombic, *Pbca*
a = 13.9100 (2) Å
b = 7.9890 (6) Å
c = 16.4080 (7) Å
V = 1823.37 (16) Å^3
Z = 8
D_x = 1.313 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 12674 reflections
θ = 1–26.3°
μ = 0.09 mm^{-1}
T = 293 (2) K
Rectangular, red
0.4 × 0.2 × 0.1 mm

Data collection

KappaCCD diffractometer
φ scans
Absorption correction: none
12674 measured reflections
1693 independent reflections
1532 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 26.3°
$h = -6 \rightarrow 17$
$k = -14 \rightarrow 8$
$l = -20 \rightarrow 0$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.225
S = 1.21
1693 reflections
118 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.1378P)^2 + 0.5336P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

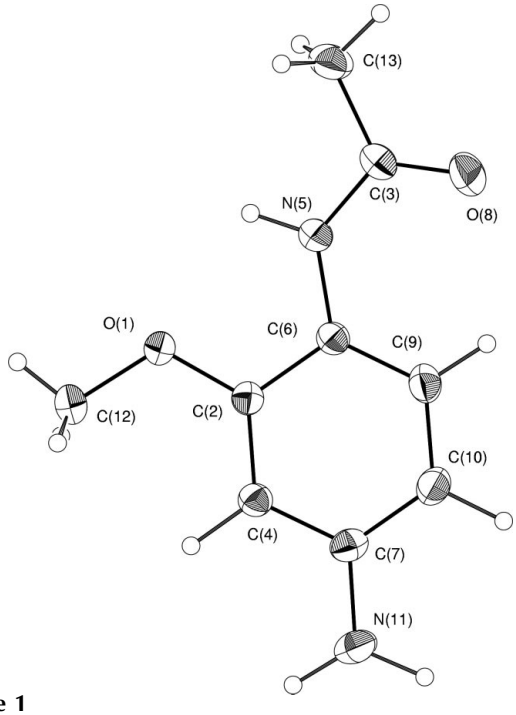


Figure 1
*ORTEP*II (Johnson, 1976) view of the title molecule, with ellipsoids plotted at the 50% probability level.

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N5—H5···O1	0.94	2.19	2.598 (2)	105
N11—H11A···O8^{i}	1.03	2.09	3.062 (3)	157
N11—H11B···O8^{ii}	1.00	2.39	3.374 (3)	168

Symmetry codes: (i) $-x, \frac{1}{2}+y, \frac{3}{2}-z$; (ii) $x, \frac{1}{2}-y, z-\frac{1}{2}$.

Data collection: *KappaCCD Software* (Nonius, 1998); data reduction: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976).

References

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