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N-(3-Pyridylmethyl)salicylamide

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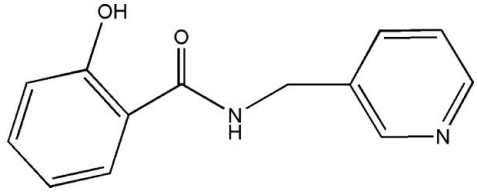
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.002 Å; R factor = 0.047; wR factor = 0.128; data-to-parameter ratio = 16.6.

In the title compound, $C_{13}H_{12}N_2O_2$, all bond lengths and angles are within normal ranges. N—H···N and C—H···N hydrogen bonding, with N···N = 2.986 (2) Å, C···N = 3.453 (2) Å, N—H···N = 160° and C—H···N = 158°, links molecules into supramolecular chains in the crystal structure.

Related literature

For related literature, see: Zhang *et al.* (2002).



Experimental

Crystal data

$C_{13}H_{12}N_2O_2$
M_r = 228.25
Orthorhombic, *Pbca*
a = 12.218 (2) Å
b = 10.928 (2) Å
c = 16.757 (3) Å
V = 2237.4 (7) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 295 (2) K
0.58 × 0.56 × 0.52 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: none
16054 measured reflections
2557 independent reflections
2359 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.128
S = 1.12
2557 reflections
154 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2B···N1^{i}	0.86	2.16	2.986 (2)	160
O2—H2A···O1	0.82	1.80	2.529 (2)	147
C9—H9···N1^{i}	0.93	2.57	3.453 (2)	158

Symmetry code: (i) $-x+\frac{5}{2}, y-\frac{1}{2}, z$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2076).

References

Bruker (1998). *SMART*, *SAINT* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
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supplementary materials

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N-(3-Pyridylmethyl)salicylamide

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Experimental

A mixture of methyl salicylate (1 mmol, 0.152 g) and 3-(aminomethyl)pyridine (1 mmol, 0.108 g) was reflux at 120 °C in 25 ml $CHCl_3$ solution for 5 h. This resulting solution was cooled and the pale yellow crystals formed. Yield: 60%, m.p.172. Anal. Calcd. for $C_{13}H_{12}N_2O_2$: C, 68.41; H, 5.30; N, 12.27; Found: C, 68.24; H, 5.23; N, 12.11%.

Refinement

H2A and H2B atoms were initially located in difference Fourier map, and were subsequently included in the refinement in calculated positions ans treated as riding atom. All atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms (C—H = 0.93, 0.97 Å; N—H = 0.86 Å; O—H = 0.82 Å) and U_{iso}(H) values weren taken to be equal to 1.2 U_{eq}(C, N) and 1.5Ueq(O).

Figures

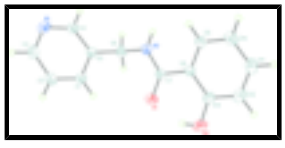

Fig. 1. The structure of (I) showing 30% probability displacement ellipsoids and the atom-numbering scheme.

N-(3-Pyridylmethyl)salicylamide

Crystal data

$C_{13}H_{12}N_2O_2$	D_x = 1.355 Mg m^{-3}
M_r = 228.25	Melting point: 172 K
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 25 reflections
a = 12.218 (2) Å	θ = 1.0–27.5º
b = 10.928 (2) Å	μ = 0.09 mm^{-1}
c = 16.757 (3) Å	*T* = 295 (2) K
V = 2237.4 (7) Å^3	Block, yellow
Z = 8	0.58 × 0.56 × 0.52 mm
F_{000} = 960	

Data collection

Bruker SMART CCD	2359 reflections with $I > 2\sigma(I)$

diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

T = 295(2) K

phi and ω scans

Absorption correction: none

16054 measured reflections

2557 independent reflections

R_{int} = 0.026

θ_{max} = 27.5º

θ_{min} = 2.4º

h = −15→12

k = −14→14

l = −20→21

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.047

$wR(F^2)$ = 0.128

S = 1.12

2557 reflections

154 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0642P)^2 + 0.3875P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.001

$\Delta\rho_{max}$ = 0.22 e Å^{-3}

$\Delta\rho_{min}$ = −0.14 e Å^{-3}

Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.87402 (8)	0.14006 (9)	0.31068 (7)	0.0549 (3)
N2	1.05351 (9)	0.09770 (9)	0.31664 (7)	0.0410 (3)
H2B	1.1047	0.0530	0.3365	0.049*
C8	0.92537 (10)	−0.03485 (11)	0.38595 (7)	0.0355 (3)
C5	1.10580 (10)	0.31634 (11)	0.30579 (7)	0.0369 (3)
C1	1.02288 (10)	0.38677 (12)	0.33848 (8)	0.0416 (3)
H1	0.9504	0.3615	0.3345	0.050*
C13	0.81588 (10)	−0.07066 (12)	0.39587 (8)	0.0439 (3)
C4	1.21143 (11)	0.35963 (12)	0.31291 (9)	0.0462 (3)
H4	1.2676	0.3132	0.2909	0.055*

N1	1.23798 (10)	0.46445 (11)	0.34950 (8)	0.0549 (3)
C7	0.94970 (10)	0.07362 (11)	0.33559 (8)	0.0380 (3)
C9	1.00574 (11)	−0.10440 (12)	0.42388 (8)	0.0432 (3)
H9	1.0788	−0.0816	0.4188	0.052*
O2	0.73213 (8)	−0.00715 (11)	0.36415 (8)	0.0688 (4)
H2A	0.7560	0.0527	0.3404	0.103*
C6	1.08250 (12)	0.19794 (12)	0.26310 (8)	0.0460 (3)
H6B	1.0229	0.2108	0.2258	0.055*
H6A	1.1466	0.1747	0.2326	0.055*
C3	1.15656 (13)	0.52891 (13)	0.38062 (9)	0.0532 (4)
H3	1.1735	0.6018	0.4065	0.064*
C12	0.79112 (12)	−0.17601 (14)	0.43906 (9)	0.0542 (4)
H12	0.7188	−0.2015	0.4434	0.065*
C2	1.04838 (12)	0.49411 (12)	0.37683 (9)	0.0481 (3)
H2	0.9939	0.5421	0.3997	0.058*
C10	0.97963 (13)	−0.20563 (13)	0.46849 (9)	0.0518 (4)
H10	1.0344	−0.2495	0.4943	0.062*
C11	0.87208 (14)	−0.24216 (14)	0.47500 (9)	0.0549 (4)
H11	0.8546	−0.3121	0.5040	0.066*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0385 (5)	0.0485 (6)	0.0778 (7)	0.0068 (4)	−0.0065 (5)	0.0142 (5)
N2	0.0351 (6)	0.0339 (5)	0.0541 (6)	0.0008 (4)	0.0023 (5)	0.0004 (4)
C8	0.0318 (6)	0.0348 (6)	0.0398 (6)	0.0001 (4)	−0.0002 (5)	−0.0050 (5)
C5	0.0357 (6)	0.0348 (6)	0.0403 (6)	−0.0009 (5)	0.0022 (5)	0.0049 (5)
C1	0.0308 (6)	0.0412 (6)	0.0529 (7)	0.0001 (5)	0.0010 (5)	0.0033 (5)
C13	0.0334 (6)	0.0484 (7)	0.0498 (7)	0.0006 (5)	−0.0005 (5)	−0.0017 (6)
C4	0.0322 (6)	0.0444 (7)	0.0620 (8)	0.0009 (5)	0.0045 (6)	0.0043 (6)
N1	0.0375 (6)	0.0505 (7)	0.0766 (8)	−0.0080 (5)	−0.0068 (6)	0.0022 (6)
C7	0.0344 (6)	0.0344 (6)	0.0453 (6)	0.0018 (5)	−0.0024 (5)	−0.0040 (5)
C9	0.0360 (6)	0.0432 (7)	0.0504 (7)	0.0025 (5)	−0.0027 (5)	−0.0009 (6)
O2	0.0306 (5)	0.0763 (8)	0.0994 (9)	0.0018 (5)	−0.0056 (5)	0.0242 (7)
C6	0.0490 (8)	0.0411 (6)	0.0478 (7)	−0.0038 (6)	0.0098 (6)	−0.0023 (5)
C3	0.0553 (9)	0.0398 (7)	0.0645 (9)	−0.0046 (6)	−0.0082 (7)	−0.0039 (6)
C12	0.0451 (8)	0.0580 (8)	0.0595 (8)	−0.0117 (6)	0.0065 (6)	0.0030 (7)
C2	0.0464 (8)	0.0398 (7)	0.0582 (8)	0.0060 (5)	0.0036 (6)	−0.0016 (6)
C10	0.0565 (9)	0.0472 (7)	0.0517 (8)	0.0072 (6)	−0.0058 (6)	0.0066 (6)
C11	0.0655 (9)	0.0491 (8)	0.0502 (8)	−0.0062 (7)	0.0048 (7)	0.0078 (6)

Geometric parameters (Å, °)

O1—C7	1.2474 (15)	C4—H4	0.9300
N2—C7	1.3337 (16)	N1—C3	1.326 (2)
N2—C6	1.4596 (16)	C9—C10	1.3727 (19)
N2—H2B	0.8600	C9—H9	0.9300
C8—C9	1.3950 (18)	O2—H2A	0.8200
C8—C13	1.4037 (17)	C6—H6B	0.9700

C8—C7	1.4851 (18)	C6—H6A	0.9700
C5—C4	1.3797 (18)	C3—C2	1.377 (2)
C5—C1	1.3852 (17)	C3—H3	0.9300
C5—C6	1.5057 (17)	C12—C11	1.365 (2)
C1—C2	1.373 (2)	C12—H12	0.9300
C1—H1	0.9300	C2—H2	0.9300
C13—O2	1.3459 (17)	C10—C11	1.378 (2)
C13—C12	1.393 (2)	C10—H10	0.9300
C4—N1	1.3391 (19)	C11—H11	0.9300
C7—N2—C6	121.68 (11)	C8—C9—H9	119.2
C7—N2—H2B	119.2	C13—O2—H2A	109.5
C6—N2—H2B	119.2	N2—C6—C5	113.50 (11)
C9—C8—C13	117.71 (12)	N2—C6—H6B	108.9
C9—C8—C7	123.56 (11)	C5—C6—H6B	108.9
C13—C8—C7	118.73 (11)	N2—C6—H6A	108.9
C4—C5—C1	117.35 (12)	C5—C6—H6A	108.9
C4—C5—C6	120.83 (12)	H6B—C6—H6A	107.7
C1—C5—C6	121.81 (11)	N1—C3—C2	123.73 (13)
C2—C1—C5	119.58 (12)	N1—C3—H3	118.1
C2—C1—H1	120.2	C2—C3—H3	118.1
C5—C1—H1	120.2	C11—C12—C13	120.63 (13)
O2—C13—C12	117.79 (12)	C11—C12—H12	119.7
O2—C13—C8	122.28 (12)	C13—C12—H12	119.7
C12—C13—C8	119.93 (12)	C1—C2—C3	118.38 (13)
N1—C4—C5	124.02 (13)	C1—C2—H2	120.8
N1—C4—H4	118.0	C3—C2—H2	120.8
C5—C4—H4	118.0	C9—C10—C11	119.89 (13)
C3—N1—C4	116.93 (12)	C9—C10—H10	120.1
O1—C7—N2	120.69 (12)	C11—C10—H10	120.1
O1—C7—C8	120.42 (11)	C12—C11—C10	120.18 (14)
N2—C7—C8	118.89 (11)	C12—C11—H11	119.9
C10—C9—C8	121.57 (13)	C10—C11—H11	119.9
C10—C9—H9	119.2		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2B···N1^{i}	0.86	2.16	2.986 (2)	160
O2—H2A···O1	0.82	1.80	2.529 (2)	147
C9—H9···N1^{i}	0.93	2.57	3.453 (2)	158

Symmetry codes: (i) −*x*+5/2, *y*−1/2, *z*.

Fig. 1