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Zwitterionic 2-{[3-(1*H*-indol-3-yl)-propenyl]methylammonio}phenolate

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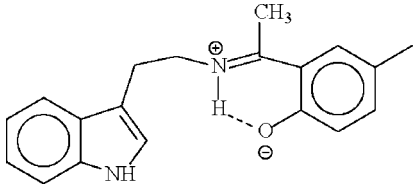
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.002 Å; R factor = 0.042; wR factor = 0.125; data-to-parameter ratio = 15.8.

The title Schiff base, $C_{19}H_{20}N_2O$, exists in its zwitterionic form, as the phenolic H atom has been transferred to the iminio group; the resulting iminium and hydroxy groups are linked by an intramolecular N—H···O hydrogen bond. Two zwitterions lie across a centre of inversion and interact through two N_{indole}—H···O hydrogen bonds to form a dimer.

Related literature

See Rodriguez *et al.* (1987) for the crystal structure of neutral 2-[2-(1*H*-indol-3-yl)ethyliminomethy]phenol (1*H*-indole-3-ethylenesalicylaldimine) and Zarza *et al.* (1988) for the crystal structure of zwitterionic 2-[2-(1*H*-indol-3-yl)ethylimino-methyl]-6-methoxyphenol.



Experimental

Crystal data

$C_{19}H_{20}N_2O$
M_r = 292.37
Monoclinic, $P2_1/n$
a = 13.5170 (2) Å
b = 8.5778 (1) Å
c = 14.4551 (2) Å
β = 114.619 (1)°
V = 1523.66 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 173 (2) K
0.35 × 0.26 × 0.21 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: none
23521 measured reflections
4406 independent reflections
3516 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.126
S = 1.01
4406 reflections
279 parameters
19 restraints
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*n*···O1	0.90 (1)	1.66 (1)	2.487 (1)	151 (2)
N2—H2*n*···O1^{i}	0.89 (1)	1.93 (1)	2.807 (1)	168 (2)

Symmetry code: (i) $-x+1, -y+1, -z+1$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2472).

References

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bruker (2005). *APEX2* (Version 2.0-2) and *SAINT* (Version 7.12a). Bruker AXS Inc., Madison, Wisconsin, USA.
Rodriguez, M. L., Medina de la Rosa, E., Gili, P., Zarza, P. M., Reyes, M. G. M., Medina, A. & Díaz González, M. C. (1987). *Acta Cryst.* C**43**, 134–136.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Westrip, S. P. (2007). *publCIF*. In preparation.
Zarza, P. M., Gill, P., Díaz González, M. C., Martin Reyes, M. G., Arrieta, J. M., Nastopoulos, V., Germain, G. & Debaerdemaeker, T. (1988). *Acta Cryst.* C**44**, 678–681.

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supplementary materials

Acta Cryst. (2007). E**63**, o3458 [**doi:10.1107/S1600536807032643**]

Zwitterionic 2-{[3-(1*H*-indol-3-yl)propenyl]methylammonio}phenolate

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Comment

Some Schiff bases that are formed from a primary amine and a substituted salicylaldehyde (or 2-hydroxyacetophenone) exist in a zwitterionic form as the phenolic hydrogen is transferred to the imino group. Among the (indol-3-yl)ethyl-2-amine derivatives that have been synthesized, the crystal structures of only two have been reported: 2-[2-(1*H*-Indol-3-yl)ethyliminomethy]phenol (1*H*-indole-3-ethylenesalicylaldimine exists as a neutral compound (Rodriguez *et al.*,1987) whereas 2-[2-(1*H*-indol-3-yl)ethylminomethyl]-6-methoxyphenol is zwitterionic (Zarza *et al.*, 1988). The title compound, (I), (Fig. 1) exists in the latter form; two zwitterions are linked by an N_{indole}–H···O hydrogen bond (Table 1) into a dimer.

Experimental

2-(Indol-3-yl)ethylamine (3.2 g, 19.9 mmol) and 2-hydroxy-5-methylacetophenone (3.0 g, 19.9 mmol) were heated in ethanol (50 ml) for 2 h. The solution was filtered; slow evaporation of the solvent yielded faint yellow blocks of (I).

Refinement

All hydrogen atoms were located in difference Fourier maps, and were refined with distance restraints C—H = 1.00±0.01 Å and N–H = 0.88±0.01 Å. Their U_{iso} values were freely refined.

Figures

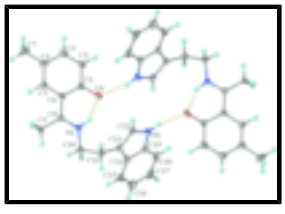

Fig. 1. View of (I) shoiwng the hydrogen-bonded dimer; displacement ellipsoids are drawn at the 70% probability level, and H atoms as spheres of arbitrary radius. The dashed lines denote hydrogen bonds. [Symmetry code *i*: 1 − *x*, 1 − *y*, 1 − *z*.]

2-{[3-(1*H*-indol-3-yl)propenyl]methylammonio}phenolate

Crystal data

$C_{19}H_{20}N_2O$	F_{000} = 624
M_r = 292.37	D_x = 1.275 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 7004 reflections
a = 13.5170 (2) Å	θ = 2.7–31.3°
b = 8.5778 (1) Å	μ = 0.08 mm^{-1}

c = 14.4551 (2) Å	T = 173 (2) K
β = 114.619 (1)º	Block, pale yellow
V = 1523.66 (4) Å^3	0.35 × 0.26 × 0.21 mm
Z = 4	

Data collection

Bruker APEXII CCD area-detector diffractometer	3516 reflections with $I > 2\sigma(I)$
Radiation source: medium-focus sealed tube	R_{int} = 0.036
Monochromator: graphite	θ_{max} = 30.0º
T = 173(2) K	θ_{min} = 1.7º
φ and ω scans	h = −19→18
Absorption correction: none	k = −12→11
23521 measured reflections	l = −20→20
4406 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.042	All H-atom parameters refined
$wR(F^2)$ = 0.126	$w = 1/[\sigma^2(F_o^2) + (0.0734P)^2 + 0.3723P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.01	$(\Delta/\sigma)_{max}$ = 0.001
4406 reflections	$\Delta\rho_{max}$ = 0.41 e Å^{-3}
279 parameters	$\Delta\rho_{min}$ = −0.23 e Å^{-3}
19 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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

	x	y	z	U_{iso}*/U_{eq}
O1	0.33096 (6)	0.49058 (9)	0.57718 (6)	0.02106 (18)
N1	0.23306 (7)	0.23687 (10)	0.53951 (7)	0.01704 (19)
N2	0.49741 (8)	0.32926 (11)	0.42664 (8)	0.0209 (2)
C1	0.25791 (9)	0.54412 (12)	0.60614 (8)	0.0171 (2)
C2	0.26495 (9)	0.69894 (12)	0.64407 (9)	0.0205 (2)
C3	0.18869 (9)	0.75560 (13)	0.67537 (9)	0.0217 (2)
C4	0.10061 (9)	0.66421 (13)	0.67272 (8)	0.0207 (2)
C5	0.09244 (9)	0.51336 (13)	0.63649 (8)	0.0187 (2)
C6	0.16864 (8)	0.45039 (12)	0.60263 (8)	0.0162 (2)
C7	0.01783 (11)	0.73171 (16)	0.70630 (10)	0.0289 (3)
C8	0.15994 (8)	0.28929 (12)	0.56854 (8)	0.0156 (2)
C9	0.07030 (9)	0.18642 (13)	0.56894 (9)	0.0208 (2)
C10	0.24093 (9)	0.07834 (12)	0.50569 (9)	0.0202 (2)

C11	0.35855 (9)	0.04142 (13)	0.52407 (9)	0.0199 (2)
C12	0.47967 (9)	0.25886 (13)	0.50420 (9)	0.0199 (2)
C13	0.40163 (9)	0.14509 (12)	0.46586 (8)	0.0176 (2)
C14	0.36938 (9)	0.14302 (12)	0.35741 (9)	0.0179 (2)
C15	0.29601 (10)	0.05272 (14)	0.27707 (9)	0.0245 (2)
C16	0.28554 (10)	0.08129 (17)	0.17906 (10)	0.0288 (3)
C17	0.34742 (10)	0.19798 (16)	0.15950 (10)	0.0280 (3)
C18	0.42114 (10)	0.28781 (14)	0.23730 (10)	0.0238 (2)
C19	0.43160 (9)	0.25923 (12)	0.33626 (9)	0.0188 (2)
H1N	0.2810 (13)	0.3128 (17)	0.5431 (15)	0.050 (5)*
H2N	0.5501 (11)	0.3947 (16)	0.4316 (12)	0.034 (4)*
H2	0.3273 (10)	0.7633 (16)	0.6463 (12)	0.031 (4)*
H3	0.1963 (13)	0.8649 (11)	0.7016 (11)	0.030 (4)*
H5	0.0309 (9)	0.4469 (15)	0.6345 (11)	0.025 (4)*
H7A	−0.0255 (14)	0.8188 (18)	0.6613 (13)	0.056 (6)*
H7C	0.0516 (13)	0.7826 (19)	0.7746 (9)	0.041 (5)*
H7B	−0.0326 (14)	0.6505 (19)	0.7118 (15)	0.059 (6)*
H9A	0.0684 (16)	0.0850 (15)	0.5364 (14)	0.058 (6)*
H9B	0.0804 (15)	0.168 (2)	0.6398 (8)	0.050 (5)*
H9C	−0.0012 (9)	0.2380 (18)	0.5348 (11)	0.037 (4)*
H10A	0.2141 (12)	0.0024 (15)	0.5416 (11)	0.030 (4)*
H10B	0.1942 (10)	0.0725 (16)	0.4313 (7)	0.019 (3)*
H11A	0.3595 (11)	−0.0698 (11)	0.5031 (11)	0.024 (4)*
H11B	0.4061 (10)	0.0464 (17)	0.5990 (7)	0.023 (4)*
H12	0.5225 (11)	0.2920 (18)	0.5761 (7)	0.028 (4)*
H15	0.2513 (11)	−0.0278 (14)	0.2920 (11)	0.027 (4)*
H16	0.2377 (15)	0.019 (2)	0.1234 (14)	0.042 (5)*
H17	0.3362 (13)	0.2144 (19)	0.0881 (8)	0.036 (4)*
H18	0.4634 (11)	0.3714 (14)	0.2233 (11)	0.028 (4)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0195 (4)	0.0183 (4)	0.0292 (4)	−0.0025 (3)	0.0139 (3)	0.0005 (3)
N1	0.0173 (4)	0.0148 (4)	0.0217 (5)	−0.0016 (3)	0.0108 (4)	0.0008 (3)
N2	0.0194 (4)	0.0180 (4)	0.0297 (5)	−0.0038 (3)	0.0145 (4)	−0.0009 (4)
C1	0.0174 (5)	0.0168 (5)	0.0157 (5)	−0.0003 (4)	0.0054 (4)	0.0030 (4)
C2	0.0211 (5)	0.0168 (5)	0.0207 (5)	−0.0025 (4)	0.0059 (4)	0.0002 (4)
C3	0.0238 (6)	0.0188 (5)	0.0170 (5)	0.0015 (4)	0.0029 (4)	−0.0017 (4)
C4	0.0198 (5)	0.0239 (5)	0.0155 (5)	0.0040 (4)	0.0045 (4)	−0.0018 (4)
C5	0.0166 (5)	0.0215 (5)	0.0173 (5)	0.0001 (4)	0.0064 (4)	−0.0012 (4)
C6	0.0159 (5)	0.0168 (4)	0.0154 (5)	−0.0003 (4)	0.0060 (4)	0.0005 (4)
C7	0.0262 (6)	0.0339 (6)	0.0265 (6)	0.0061 (5)	0.0108 (5)	−0.0076 (5)
C8	0.0149 (5)	0.0177 (5)	0.0143 (5)	−0.0015 (3)	0.0061 (4)	0.0007 (4)
C9	0.0189 (5)	0.0214 (5)	0.0262 (6)	−0.0056 (4)	0.0133 (5)	−0.0043 (4)
C10	0.0209 (5)	0.0152 (5)	0.0294 (6)	−0.0022 (4)	0.0155 (5)	−0.0013 (4)
C11	0.0204 (5)	0.0172 (5)	0.0265 (6)	0.0019 (4)	0.0142 (5)	0.0033 (4)
C12	0.0181 (5)	0.0191 (5)	0.0249 (6)	0.0001 (4)	0.0114 (4)	−0.0012 (4)

C13	0.0161 (5)	0.0162 (4)	0.0232 (5)	0.0008 (4)	0.0110 (4)	0.0004 (4)
C14	0.0160 (5)	0.0172 (5)	0.0234 (5)	0.0008 (4)	0.0110 (4)	0.0008 (4)
C15	0.0206 (5)	0.0267 (6)	0.0281 (6)	−0.0033 (4)	0.0120 (5)	−0.0040 (5)
C16	0.0236 (6)	0.0374 (7)	0.0249 (6)	0.0004 (5)	0.0095 (5)	−0.0059 (5)
C17	0.0274 (6)	0.0370 (7)	0.0239 (6)	0.0099 (5)	0.0148 (5)	0.0036 (5)
C18	0.0231 (5)	0.0252 (5)	0.0300 (6)	0.0061 (4)	0.0179 (5)	0.0065 (5)
C19	0.0165 (5)	0.0172 (5)	0.0261 (6)	0.0023 (4)	0.0122 (4)	0.0018 (4)

Geometric parameters (Å, °)

O1—C1	1.3059 (13)	C9—H9A	0.984 (9)
N1—C8	1.3041 (13)	C9—H9B	0.989 (9)
N1—C10	1.4638 (14)	C9—H9C	0.988 (9)
N1—H1N	0.905 (9)	C10—C11	1.5319 (15)
N2—C19	1.3750 (15)	C10—H10A	0.991 (9)
N2—C12	1.3795 (15)	C10—H10B	0.995 (8)
N2—H2N	0.886 (9)	C11—C13	1.4986 (14)
C1—C2	1.4247 (15)	C11—H11A	1.003 (9)
C1—C6	1.4332 (14)	C11—H11B	1.004 (8)
C2—C3	1.3755 (16)	C12—C13	1.3730 (15)
C2—H2	0.997 (9)	C12—H12	0.998 (9)
C3—C4	1.4127 (16)	C13—C14	1.4418 (16)
C3—H3	1.001 (9)	C14—C15	1.4045 (16)
C4—C5	1.3830 (15)	C14—C19	1.4173 (14)
C4—C7	1.5085 (16)	C15—C16	1.3856 (18)
C5—C6	1.4185 (14)	C15—H15	0.999 (9)
C5—H5	0.998 (8)	C16—C17	1.4066 (19)
C6—C8	1.4553 (14)	C16—H16	0.959 (19)
C7—H7A	1.003 (9)	C17—C18	1.3848 (19)
C7—H7C	0.999 (9)	C17—H17	0.989 (9)
C7—H7B	1.001 (9)	C18—C19	1.3992 (16)
C8—C9	1.5009 (14)	C18—H18	0.989 (9)
C8—N1—C10	126.73 (9)	H9B—C9—H9C	105.9 (14)
C8—N1—H1N	110.7 (12)	N1—C10—C11	110.41 (9)
C10—N1—H1N	122.5 (12)	N1—C10—H10A	110.0 (9)
C19—N2—C12	108.56 (9)	C11—C10—H10A	110.7 (9)
C19—N2—H2N	122.2 (10)	N1—C10—H10B	107.8 (8)
C12—N2—H2N	128.2 (11)	C11—C10—H10B	108.8 (8)
O1—C1—C2	120.86 (10)	H10A—C10—H10B	109.1 (12)
O1—C1—C6	121.95 (9)	C13—C11—C10	113.45 (9)
C2—C1—C6	117.18 (10)	C13—C11—H11A	109.7 (8)
C3—C2—C1	121.13 (10)	C10—C11—H11A	106.7 (8)
C3—C2—H2	122.2 (9)	C13—C11—H11B	110.9 (8)
C1—C2—H2	116.7 (9)	C10—C11—H11B	109.3 (8)
C2—C3—C4	122.25 (10)	H11A—C11—H11B	106.5 (12)
C2—C3—H3	118.9 (9)	C13—C12—N2	110.34 (10)
C4—C3—H3	118.9 (9)	C13—C12—H12	129.6 (9)
C5—C4—C3	117.57 (10)	N2—C12—H12	120.0 (9)
C5—C4—C7	121.88 (11)	C12—C13—C14	106.32 (9)

C3—C4—C7	120.53 (10)	C12—C13—C11	127.45 (10)
C4—C5—C6	122.15 (10)	C14—C13—C11	126.22 (10)
C4—C5—H5	118.6 (8)	C15—C14—C19	119.18 (10)
C6—C5—H5	119.2 (8)	C15—C14—C13	134.06 (10)
C5—C6—C1	119.72 (10)	C19—C14—C13	106.74 (9)
C5—C6—C8	120.70 (9)	C16—C15—C14	118.95 (11)
C1—C6—C8	119.53 (9)	C16—C15—H15	122.0 (9)
C4—C7—H7A	112.8 (11)	C14—C15—H15	119.0 (9)
C4—C7—H7C	113.0 (10)	C15—C16—C17	121.02 (12)
H7A—C7—H7C	102.6 (15)	C15—C16—H16	120.3 (10)
C4—C7—H7B	112.3 (12)	C17—C16—H16	118.6 (10)
H7A—C7—H7B	109.7 (16)	C18—C17—C16	121.31 (11)
H7C—C7—H7B	105.8 (15)	C18—C17—H17	120.9 (10)
N1—C8—C6	118.11 (9)	C16—C17—H17	117.8 (10)
N1—C8—C9	121.33 (9)	C17—C18—C19	117.69 (11)
C6—C8—C9	120.56 (9)	C17—C18—H18	121.3 (9)
C8—C9—H9A	112.2 (11)	C19—C18—H18	121.0 (9)
C8—C9—H9B	109.7 (11)	N2—C19—C18	130.14 (10)
H9A—C9—H9B	108.4 (15)	N2—C19—C14	108.02 (10)
C8—C9—H9C	111.0 (10)	C18—C19—C14	121.84 (11)
H9A—C9—H9C	109.4 (15)		
O1—C1—C2—C3	−179.52 (10)	N2—C12—C13—C14	0.69 (12)
C6—C1—C2—C3	−0.33 (16)	N2—C12—C13—C11	−179.97 (10)
C1—C2—C3—C4	0.63 (17)	C10—C11—C13—C12	109.95 (13)
C2—C3—C4—C5	−0.39 (17)	C10—C11—C13—C14	−70.83 (14)
C2—C3—C4—C7	−179.08 (11)	C12—C13—C14—C15	178.40 (12)
C3—C4—C5—C6	−0.14 (16)	C11—C13—C14—C15	−1.0 (2)
C7—C4—C5—C6	178.53 (11)	C12—C13—C14—C19	−0.10 (12)
C4—C5—C6—C1	0.41 (16)	C11—C13—C14—C19	−179.45 (10)
C4—C5—C6—C8	177.68 (10)	C19—C14—C15—C16	−0.83 (17)
O1—C1—C6—C5	179.00 (9)	C13—C14—C15—C16	−179.19 (12)
C2—C1—C6—C5	−0.17 (15)	C14—C15—C16—C17	0.36 (19)
O1—C1—C6—C8	1.71 (16)	C15—C16—C17—C18	0.27 (19)
C2—C1—C6—C8	−177.47 (9)	C16—C17—C18—C19	−0.38 (18)
C10—N1—C8—C6	178.04 (10)	C12—N2—C19—C18	−179.07 (11)
C10—N1—C8—C9	−0.81 (17)	C12—N2—C19—C14	0.95 (12)
C5—C6—C8—N1	−179.09 (10)	C17—C18—C19—N2	179.90 (11)
C1—C6—C8—N1	−1.83 (15)	C17—C18—C19—C14	−0.12 (16)
C5—C6—C8—C9	−0.23 (15)	C15—C14—C19—N2	−179.29 (10)
C1—C6—C8—C9	177.03 (10)	C13—C14—C19—N2	−0.52 (12)
C8—N1—C10—C11	−154.48 (10)	C15—C14—C19—C18	0.73 (16)
N1—C10—C11—C13	−62.04 (13)	C13—C14—C19—C18	179.49 (10)
C19—N2—C12—C13	−1.04 (13)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1N···O1	0.90 (1)	1.66 (1)	2.487 (1)	151 (2)
N2—H2N···O1^{i}	0.89 (1)	1.93 (1)	2.807 (1)	168 (2)

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

Fig. 1