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## Key indicators

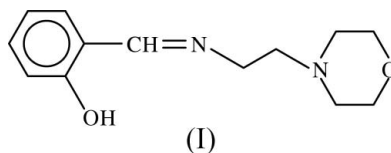
Single-crystal X-ray study  
 $T = 100\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.002\text{ \AA}$   
 $R$  factor = 0.032  
 $wR$  factor = 0.085  
Data-to-parameter ratio = 9.0For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.*(E)*-2-[(2-Morpholinoethylimino)methyl]phenolThe title compound,  $\text{C}_{13}\text{H}_{18}\text{N}_2\text{O}_2$ , exists in the enol-imine tautomeric form with a strong intramolecular  $\text{O}-\text{H}\cdots\text{N}$  hydrogen bond [ $\text{O}\cdots\text{N} = 2.5795(18)\text{ \AA}$ ], and the morpholine ring adopts an almost perfect chair conformation.

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## Comment

Schiff bases are widely used as ligands in the field of coordination chemistry (Calligaris & Randaccio, 1987) and they are important in diverse areas of chemistry because of their biological activities (Lozier *et al.*, 1975; Garnovskii *et al.*, 1993; Costamagna *et al.*, 1992; Walsh & Orme-Johnson, 1987). *o*-Hydroxy Schiff bases derived from the reaction of *o*-hydroxyaldehydes with aniline have been extensively examined (Stewart & Lingafelter, 1959; Calligaris *et al.*, 1972; Maslen & Waters, 1975). *N*-Substituted *o*-hydroxyimines have been reported to display thermochromism and photochromism in the solid state by H-atom transfer from the hydroxy O atom to the N atom (Hadjoudis *et al.*, 1987; Xu *et al.*, 1994).There are two types of intramolecular hydrogen bonds in Schiff bases, viz. keto-amine ( $\text{N}-\text{H}\cdots\text{O}$ ) and enol-imine ( $\text{N}\cdots\text{H}-\text{O}$ ) tautomeric forms. In the title compound, (I), it is seen that the enol-imine tautomer is favoured over the keto-amine tautomer. *o*-Hydroxy Schiff bases have been observed previously in the keto form (Hökelek *et al.*, 2000; Koşar *et al.*, 2004), in the enol form (Ünver *et al.*, 2002; Odabaşoğlu *et al.*, 2005) or in enol/keto mixtures (Nazır *et al.*, 2000) by means of H-atom transfer.

The molecular structure of (I) is shown in Fig. 1. Selected bond lengths and angles are listed in Table 1. The C1—O1 and

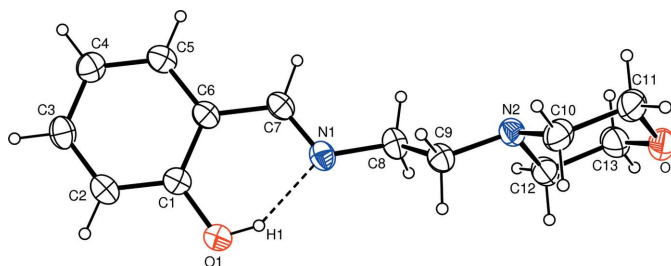


Figure 1

A view of (I), showing 50% probability displacement ellipsoids. The dashed line indicates a hydrogen bond.

C7–N1 bond lengths verify the enol–imine form of (I), and these distances are similar to other values reported in the literature [1.357 (2) and 1.287 (2) Å (Albayrak *et al.*, 2005); 1.346 (4) and 1.270 (5) Å (Şahin *et al.*, 2005)].

There is a strong intramolecular O–H···N hydrogen bond in (I) (Table 2), which is a common feature of *o*-hydroxy-salicylidene systems (Filarowski *et al.*, 2003; Yıldız *et al.*, 1998).

The morpholine ring in (I) adopts an almost perfect chair conformation, with a total puckering amplitude of  $Q_T = 0.5747$  (15) Å (Cremer & Pople, 1975). The bond distances and angles in the morpholine rings are as expected.

## Experimental

Compound (I) was prepared by refluxing a mixture of a solution containing salicylaldehyde (0.5 g 4.1 mmol) in ethanol (20 ml) and a solution containing 4-(2-aminoethyl)morpholine (0.53 g 4.1 mmol) in ethanol (20 ml). The reaction mixture was stirred for 1 h under reflux. The resulting yellow precipitate was filtered off and crystals of (I) suitable for X-ray analysis were obtained from ethyl acetate by slow evaporation (yield 93%, m.p. 318–319 K).

### Crystal data

$C_{13}H_{18}N_2O_2$	Mo $K\alpha$ radiation
$M_r = 234.29$	Cell parameters from 8146 reflections
Orthorhombic, $P2_12_12_1$	$\theta = 1.8$ – $27.2^\circ$
$a = 5.8324$ (4) Å	$\mu = 0.09$ mm $^{-1}$
$b = 9.1911$ (6) Å	$T = 100$ K
$c = 23.042$ (2) Å	Prism, yellow
$V = 1235.17$ (17) Å $^3$	$0.60 \times 0.52 \times 0.42$ mm
$Z = 4$	
$D_x = 1.260$ Mg m $^{-3}$	

### Data collection

Stoe IPDS-II diffractometer	$R_{int} = 0.045$
$\omega$ scans	$\theta_{max} = 26.0^\circ$
Absorption correction: none	$h = -7 \rightarrow 7$
6052 measured reflections	$k = -11 \rightarrow 11$
1447 independent reflections	$l = -25 \rightarrow 28$
1358 reflections with $I > 2\sigma(I)$	

### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0533P)^2 + 0.0683P]$
$R[F^2 > 2\sigma(F^2)] = 0.032$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.085$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.12$	$\Delta\rho_{max} = 0.20$ e Å $^{-3}$
1447 reflections	$\Delta\rho_{min} = -0.19$ e Å $^{-3}$
160 parameters	Extinction correction: <i>SHELXL97</i>
H atoms treated by a mixture of independent and constrained refinement	Extinction coefficient: 0.063 (6)

**Table 1**

Selected geometric parameters (Å, °).

C1–O1	1.348 (2)	C10–N2	1.460 (2)
C7–N1	1.272 (2)	C11–O2	1.420 (2)
C8–N1	1.457 (2)	C12–N2	1.463 (2)
C9–N2	1.458 (2)	C13–O2	1.426 (2)
O1–C1–C6	121.36 (14)	N2–C9–C8	110.83 (13)
N1–C7–C6	121.62 (15)	C7–N1–C8	118.41 (14)

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1–H1···N1	0.82	1.85	2.5795 (18)	148

In the absence of significant anomalous dispersion effects, 990 Friedel pairs were merged before the refinement, and the assignment of absolute configuration is arbitrary. All H atoms (except for H7) were positioned geometrically and treated using a riding model, fixing the aromatic C–H distances at 0.93 Å, the methylene C–H distances at 0.97 Å and the O–H distance at 0.82 Å [ $U_{iso}(H) = 1.2U_{eq}(C)$  and  $1.5U_{eq}(O)$ ]. Atom H7, attached to C7, was refined independently with an isotropic displacement parameter.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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## References

- Albayrak, Ç., Odabaşoğlu, M. & Büyükgüngör, O. (2005). *Acta Cryst.* **E61**, o423–o424.
- Calligaris, M., Nardin, G. & Randaccio, L. (1972). *Coord. Chem. Rev.* **7**, 385–403.
- Calligaris, M. & Randaccio, L. (1987). *Comprehensive Coordination Chemistry*, Vol. 2, edited by G. Wilkinson, pp. 715–738. London: Pergamon.
- Costamagna, J., Vargas, J., Latorre, R., Alvarado, A. & Mena, G. (1992). *Coord. Chem. Rev.* **119**, 67–68.
- Cremer, D. & Pople, J. A. (1975). *J. Am. Chem. Soc.* **97**, 1354–1358.
- Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
- Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
- Filarowski, A., Koll, A. & Glowia, T. (2003). *J. Mol. Struct.* **644**, 187–195.
- Garnovskii, A. D., Nivorozhkin, A. L. & Minkin, V. I. (1993). *Coord. Chem. Rev.* **126**, 1–69.
- Hadjoudis, E., Vitterakis, M. & Mavridis, I. M. (1987). *Tetrahedron*, **43**, 1345–1360.
- Hökelek, T., Kılıç, Z., Işıklan, M. & Toy, M. (2000). *J. Mol. Struct.* **523**, 61–69.
- Koşar, B., Büyükgüngör, O., Albayrak, Ç. & Odabaşoğlu, M. (2004). *Acta Cryst.* **C60**, o458–o460.
- Lozier, R., Bogomolni, R. A. & Stoekenius, W. (1975). *J. Biophys.* **15**, 955–962.
- Maslen, H. S. & Waters, T. N. (1975). *Coord. Chem. Rev.* **17**, 137–176.
- Nazır, H., Yıldız, M., Yılmaz, H., Tahir, M. N. & Ülkü, D. (2000). *J. Mol. Struct.* **524**, 241–250.
- Odabaşoğlu, M., Albayrak, Ç. & Büyükgüngör, O. (2005). *Acta Cryst.* **E61**, o425–o426.
- Şahin, O., Büyükgüngör, O., Albayrak, Ç. & Odabaşoğlu, M. (2005). *Acta Cryst.* **E61**, o1288–o1290.
- Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
- Stewart, J. M. & Lingafelter, E. C. (1959). *Acta Cryst.* **12**, 842–845.
- Stoe & Cie (2002). *X-AREA* and *X-RED*. Stoe & Cie, Darmstadt, Germany.
- Ünver, H., Yıldız, M., Zengin, D. M., Özbey, S. & Kendi, E. (2002). *J. Chem. Crystallogr.* **31**, 211–216.
- Walsh, C. T. & Orme-Johnson, W. H. (1987). *Biochemistry*, **26**, 4901–4906.
- Xu, X., You, X., Sun, Z., Wang, X. & Liu, H. (1994). *Acta Cryst.* **C50**, 1169–1171.
- Yıldız, M., Kılıç, Z. & Hökelek, T. (1998). *J. Mol. Struct.* **441**, 1–10.