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2-[(1,3-Benzothiazol-2-yl)iminomethyl]-6-methoxyphenol: a new monoclinic polymorph

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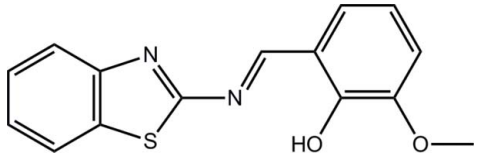
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.036; wR factor = 0.095; data-to-parameter ratio = 16.3.

The title compound, $C_{15}H_{12}N_2O_2S$, is a $P2_1/c$ polymorph of a previously reported $P2_1/n$ polymorph [Büyükgüngör *et al.* (2004). *Acta Cryst.* E**60**, o1414–o1416]. The dihedral angle between the benzothiazole (r.m.s. deviation = 0.010 Å) and the benzene ring of 7.86 (6)° compares with 10.76 (10)° in the literature structure. The methoxy substituent is almost coplanar with the benzene ring to which it is attached [C—O—C—C torsion angle = 178.31 (14)°] and the conformation about the imine bond [1.287 (2) Å] is *E*. There is an intramolecular O—H···N hydrogen bond and the hydroxy O and thioether S atoms are *syn*. In the crystal, columns are formed along the *b* axis as centrosymmetric dimeric aggregates, mediated by C—H···O interactions and linked by π–π interactions between the thiazole and benzene rings [centroid-to-centroid distance = 3.8256 (10) Å].

Related literature

For background to the biological activity of organotin compounds with N-, O- and S-atom donors, see: Affan *et al.* (2009). For the structure of the $P2_1/n$ polymorph, see: Büyükgüngör *et al.* (2004).



Experimental

Crystal data

$C_{15}H_{12}N_2O_2S$
M_r = 284.33
Monoclinic, $P2_1/c$
a = 11.6697 (11) Å
b = 6.0250 (6) Å
c = 18.6441 (18) Å
β = 94.346 (1)°
V = 1307.1 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.25 mm^{-1}
T = 100 K
0.20 × 0.16 × 0.15 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.669, T_{max} = 0.746
15750 measured reflections
2983 independent reflections
2404 reflections with $I > 2\sigma(I)$
R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.095
S = 1.05
2983 reflections
183 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1O···N2	0.84	1.88	2.6167 (17)	146
C6—H6···O2^{i}	0.95	2.56	3.424 (2)	151

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

Data collection: *SMART* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012), *QMol* (Gans & Shalloway, 2001) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2623).

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