Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-(*N*,*N*-Dimethylaminomethyl)-4-hydroxy-4-(4-chlorophenyl)thiazoline

Daniel E. Lynch[a]* and Ian McClenaghan[b]

[a]School of Science and the Environment, Coventry University, Coventry CV1 5FB, England, and [b]Key Organics Ltd, Highfield Industrial Estate, Camelford, Cornwall PL32 9QZ, England

Correspondence e-mail: apx106@coventry.ac.uk

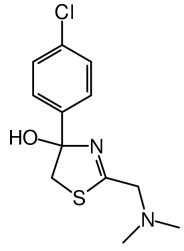
Received 22 May 2002
Accepted 28 May 2002
Online 8 June 2002

The structure of the title compound, $C_{12}H_{15}ClN_2OS$, comprises a twisted molecule that forms dimers in the solid state *via* the O—H···N(thiazole) hydrogen-bonding interaction. The phenyl ring is twisted by 88.65 (9)° with respect to the mean plane of the thiazoline ring (largest ring deviation <0.05 Å). No close contacts are observed involving the amino N atom, but one of the *N*-methyl C atoms is 3.367 (3) Å from an adjacent Cl atom, although none of the *N*-methyl H atoms are appropriately positioned to form a C—H···Cl close contact.

Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.003 Å
R factor = 0.044
wR factor = 0.147
Data-to-parameter ratio = 17.8

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



(I)

Experimental

The title compound was obtained from Key Organics Ltd and crystals were grown from an ethanol solution.

Crystal data

$C_{12}H_{15}ClN_2OS$
M_r = 270.77
Triclinic, $P\overline{1}$
a = 6.1186 (8) Å
b = 9.3865 (9) Å
c = 11.977 (2) Å
α = 103.473 (4)°
β = 97.274 (5)°
γ = 93.32 (1)°
V = 660.8 (1) Å^3
Z = 2
D_x = 1.361 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 25743 reflections
θ = 1.0–27.5°
μ = 0.43 mm^{-1}
T = 120 (2) K
Needle, colourless
0.34 × 0.07 × 0.04 mm

Data collection

Bruker–Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.867, T_{max} = 0.983
8739 measured reflections
2846 independent reflections
2206 reflections with $I > 2\sigma(I)$
R_{int} = 0.042
θ_{max} = 27.5°
h = −7 → 7
k = −12 → 12
l = −15 → 15

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.147
S = 1.01
2846 reflections
160 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O41—H41···N3^{i}	0.91 (3)	1.86 (3)	2.767 (2)	176 (3)
C21—H22···O41^{ii}	0.99	2.38	3.294 (2)	153
C42—H42···O41	0.95	2.43	2.793 (3)	102

Symmetry codes: (i) $1-x, 1-y, 2-z$; (ii) $x-1, y, z$.

All H atoms were included in the refinement, at calculated positions, as riding models, with C—H set to 0.93 (Ar—H) and 0.96 Å (CH_3), except for the O—H atom, which was located in a difference synthesis, and whose positional and displacement parameters were refined.

Data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON*97 (Spek, 1997); software used to prepare material for publication: *SHELXL*97.

The authors thank the EPSRC National Crystallography Service (Southampton).

References

Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–37.
Hooft, R. (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Spek, A. L. (1997). *PLATON*97. Version of May 1997. University of Utrecht, The Netherlands.

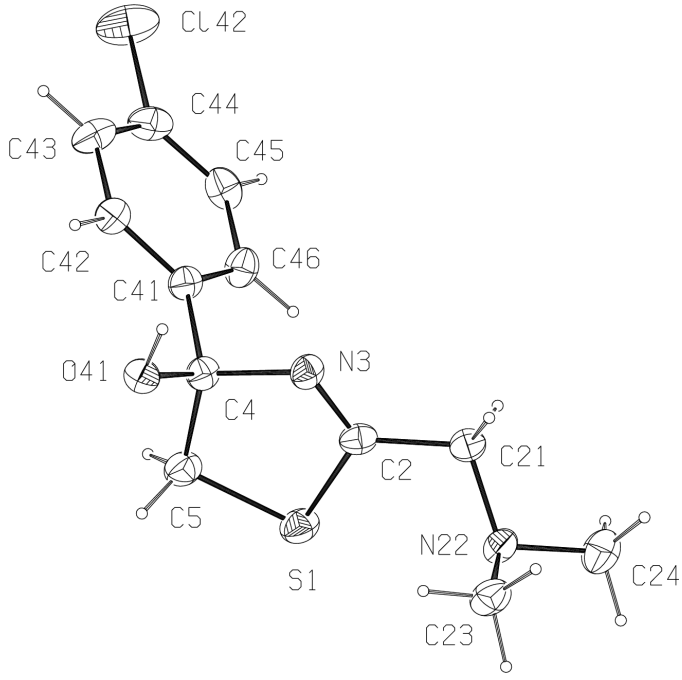


Figure 1
The molecular configuration and atom-numbering scheme for the title compound, showing 50% probability ellipsoids.