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N-(2-Chloro-4-nitrophenyl)-*N*′-octanoylthiourea

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.050
wR factor = 0.128
Data-to-parameter ratio = 14.9

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

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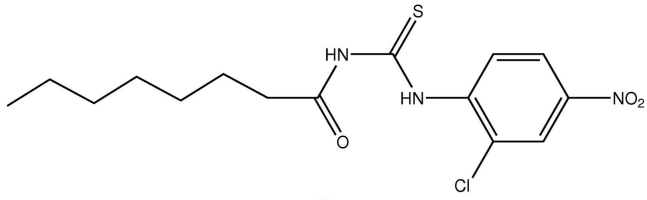
The title compound, $C_{15}H_{20}ClN_3O_3S$, adopts a *trans–cis* configuration with respect to the positions of the octanoyl and 2-chloro-4-nitrophenyl groups relative to the S atom across their respective C—N bonds. Molecules exhibit intramolecular N—H···O hydrogen bonds and are linked into dimers through N—H···S interactions.

Comment

The title compound, (I), is similar to *N*-hexanoyl-*N*′-(6-methyl-2-pyridyl)thiourea (Yusof *et al.*, 2007), except that the hexanoyl and 6-methyl-2-pyridyl groups are replaced by octanoyl and 2-chloro-4-nitrophenyl, respectively (Fig. 1). The molecule maintains a *trans–cis* configuration with respect to the position of the octanoyl and 2-chloro-4-nitrophenyl groups relative to atom S1 across the C9—N1 and C9—N2 bonds, respectively.



(I)

The bond lengths and angles are within normal ranges (Allen *et al.*, 1987) and are comparable to those in the hexanoyl/6-methyl-2-pyridyl derivative. The thiourea fragment (S1/C9/N1/N2) makes a dihedral angle of 26.6 (2)° with the mean plane of the benzene ring (C10–C15). Molecules exhibit intramolecular N—H···O hydrogen bonds (Table 1 and Fig. 1) and are linked into dimers through N—H···S interactions.

Experimental

2-Chloro-4-nitroaniline (2.12 g, 12 mmol) in 20 ml acetone was added dropwise to a stirred solution of octanoyl chloride (2.0 g, 12 mmol) and ammonium thiocyanate (0.91 g, 12 mmol) in acetone (75 ml). The mixture was refluxed for 1 h then poured onto ice. The resulting white precipitate was filtered, washed with distilled water and cold ethanol, then dried under vacuum. Single crystals were obtained by recrystallization from acetonitrile (yield: 2.13 g, 72%).

Crystal data

$C_{15}H_{20}ClN_3O_3S$
M_r = 357.85
Monoclinic, $P2_1/c$
a = 12.737 (4) Å
b = 9.355 (3) Å
c = 15.992 (5) Å
β = 111.960 (5)°
V = 1767.3 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.35 mm^{-1}
T = 298 (2) K
0.35 × 0.25 × 0.24 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.887, T_{max} = 0.921
8878 measured reflections
3105 independent reflections
2311 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.128
S = 1.03
3105 reflections
209 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O1	0.86	1.89	2.608 (3)	140
N1—H1D···S1^{i}	0.86	2.66	3.504 (3)	168

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

H atoms were visible in difference Fourier maps, but were positioned geometrically and allowed to ride, with C—H = 0.93–0.97 Å or N—H = 0.86 Å and U_{iso}(H) = 1.2U_{eq}(C,N) or 1.5U_{eq}(methyl C).

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

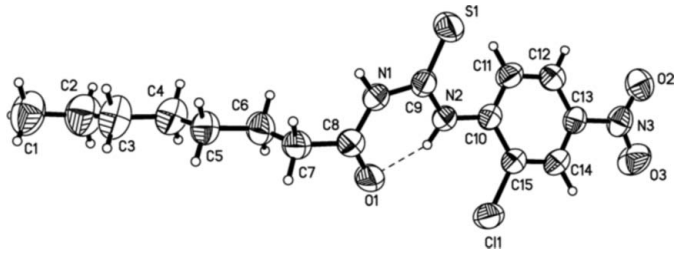


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level. The dashed line indicates an N—H···O hydrogen bond.

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