Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N-(4-Chloro-3-methylphenyl)succinamic acid

U. Chaithanya,[a] Sabine Foro[b] and B. Thimme Gowda[a]*

[a]Department of Chemistry, Mangalore University, Mangalagangotri 574 199, Mangalore, India, and [b]Institute of Materials Science, Darmstadt University of Technology, Petersenstrasse 23, D-64287 Darmstadt, Germany
Correspondence e-mail: gowdabt@yahoo.com

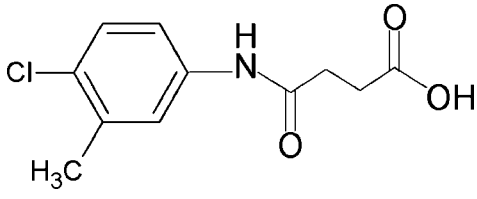
Received 25 May 2012; accepted 29 May 2012

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.008 Å; R factor = 0.090; wR factor = 0.155; data-to-parameter ratio = 12.8.

The title compound, $C_{11}H_{12}ClNO_3$, crystallizes with two independent molecules in the asymmetric unit in which the dihedral angles between the benzene ring and the amide group are 55.0 (2) and 28.2 (3)°. The two independent molecules are linked by an N—H···O hydrogen bond. In the crystal, molecules form inversion dimers *via* pairs of O—H···O hydrogen bonds. These dimers are linked into sheets parallel to $(11\bar{3})$ *via* N—H···O hydrogen bonds.

Related literature

For our studies on the effects of substituents on the structures and other aspects of *N*-(aryl)-amides, see: Gowda *et al.* (2000); Chaithanya *et al.* (2012), of *N*-chloroarylamides, see: Gowda & Rao (1989); Jyothi & Gowda (2004) and of *N*-bromoarylsulfonamides, see: Gowda & Mahadevappa (1983); Usha & Gowda (2006).



Experimental

Crystal data

$C_{11}H_{12}ClNO_3$
M_r = 241.67
Triclinic, $P\bar{1}$
a = 6.6253 (8) Å
b = 7.9634 (9) Å
c = 21.545 (3) Å
α = 88.57 (1)°
β = 81.99 (1)°
γ = 84.25 (1)°
V = 1119.9 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.33 mm^{-1}
T = 293 K
0.48 × 0.16 × 0.03 mm

Data collection

Oxford Diffraction Xcalibur diffractometer with a Sapphire CCD detector
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2009)
T_{min} = 0.857, T_{max} = 0.990
6984 measured reflections
3864 independent reflections
2640 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.090
$wR(F^2)$ = 0.155
S = 1.33
3864 reflections
303 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3*O*···O2^{i}	0.82 (2)	1.85 (2)	2.668 (5)	176 (7)
N1—H1*N*···O4^{ii}	0.86 (2)	2.09 (2)	2.934 (5)	169 (5)
O6—H6*O*···O5^{iii}	0.82 (2)	1.86 (2)	2.685 (6)	177 (8)
N2—H2*N*···O1	0.85 (2)	2.12 (2)	2.944 (6)	163 (5)

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2009); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

BTG thanks the University Grants Commission, Government of India, New Delhi, for a special grant under the UGC–BSR one-time grant to faculty.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5936).

References

Chaithanya, U., Foro, S. & Gowda, B. T. (2012). *Acta Cryst.* E**68**, o835.
Gowda, B. T., Kumar, B. H. A. & Fuess, H. (2000). *Z. Naturforsch. Teil A*, **55**, 721–728.
Gowda, B. T. & Mahadevappa, D. S. (1983). *Talanta*, **30**, 359–362.
Gowda, B. T. & Rao, P. J. M. (1989). *Bul. Chem. Soc. Jpn*, **62**, 3303–3310.
Jyothi, K. & Gowda, B. T. (2004). *Z. Naturforsch. Teil A*, **59**, 64–68.
Oxford Diffraction (2009). *CrysAlis CCD* and *CrysAlis RED*. Oxford Diffraction Ltd, Yarnton, England.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Usha, K. M. & Gowda, B. T. (2006). *J. Chem. Sci.* **118**, 351–359.