

3-(1,3-Benzodioxol-5-yl)-*N*-(2-methylpropyl)-prop-2-enamide (fagaramide)

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## Key indicators

Single-crystal X-ray study

 $T = 298$  KMean  $\sigma(\text{C}-\text{C}) = 0.002$  Å $R$  factor = 0.043 $wR$  factor = 0.134

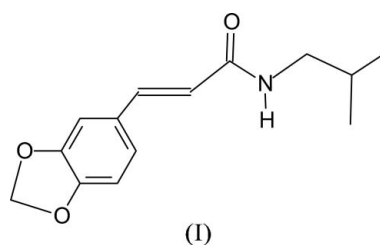
Data-to-parameter ratio = 17.5

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

The title compound,  $\text{C}_{14}\text{H}_{17}\text{NO}_3$ , is a natural product which can be isolated from many plants. In the molecule, the amide group adopts a planar *Z* geometry.

## Comment

Many plants contain the alkaloid fagaramide (Taubock & Winterstein, 1933), (I), which has been shown to be a pharmaceutically active agent in many natural products (Adesina & Reisch, 1988). Although it is well known in terms of composition (Thoms & Thumen, 1912), its structure has not been reported. We describe here the room-temperature crystal structure of (I).



In the molecular structure of (I) (Fig. 1), there is a *trans* or *E* arrangement of substituents around the styryl bond and the amide group adopts a *Z* geometry. Comparison of the amide bond lengths in the Cambridge Structural Database (Version 5.27; Allen, 2002) for the 22 entries with the fragment corresponding to a secondary cinnamoylamide reveals that, while the styryl bond length  $\text{C}6-\text{C}7$  in (I) is close to average values, the amide  $\text{C}=\text{O}$  and  $\text{C}-\text{N}$  bond lengths,  $\text{C}5=\text{O}1$  and  $\text{C}5-\text{N}1$ , are slightly longer and shorter than the average values of 1.227 and 1.357 Å, respectively. This suggests a slightly stronger amide interaction in (I), but this requires spectroscopic verification.

## Experimental

Compound (I) was isolated from *Garcinia lucida* by the methods of Goodson (1921) and Thoms & Thumen (1912) and recrystallized as long colorless prisms from a mixture of hexane and ethyl acetate (7:3).

## Crystal data

 $\text{C}_{14}\text{H}_{17}\text{NO}_3$  $M_r = 247.29$ Monoclinic,  $P2_1/n$  $a = 8.618$  (6) Å $b = 9.213$  (6) Å $c = 16.785$  (11) Å $\beta = 93.637$  (8)° $V = 1330.0$  (15) Å<sup>3</sup> $Z = 4$  $D_x = 1.235$  Mg m<sup>-3</sup> $D_m = 1.22$  Mg m<sup>-3</sup> $D_m$  measured by flotationMo  $K\alpha$  radiation $\mu = 0.09$  mm<sup>-1</sup> $T = 298$  (2) K

Prism, colorless

0.30 × 0.20 × 0.15 mm

Data collection

Bruker SMART CCD  
diffractometer  
 $\varphi$  and  $\omega$  scans  
Absorption correction: multi-scan  
(SADABS; Siemens, 1996)  
 $T_{\min} = 0.965$ ,  $T_{\max} = 0.990$

11058 measured reflections  
2856 independent reflections  
2025 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.031$   
 $\theta_{\text{max}} = 26.9^\circ$

Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.043$   
 $wR(F^2) = 0.134$   
 $S = 1.04$   
2856 reflections  
163 parameters  
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0783P)^2 + 0.0729P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.15 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.21 \text{ e } \text{\AA}^{-3}$

Table 1

Selected bond lengths ( $\text{\AA}$ ).

|        |             |         |           |
|--------|-------------|---------|-----------|
| O1—C5  | 1.239 (2)   | C8—C9   | 1.408 (2) |
| N1—C5  | 1.3338 (19) | C9—C10  | 1.365 (2) |
| N1—C4  | 1.4513 (19) | C10—O3  | 1.374 (2) |
| C1—C3  | 1.532 (2)   | C10—C11 | 1.381 (2) |
| C2—C3  | 1.508 (3)   | C11—O2  | 1.367 (2) |
| C3—C4  | 1.528 (3)   | C11—C12 | 1.364 (2) |
| C5—C6  | 1.486 (2)   | C12—C13 | 1.394 (2) |
| C6—C7  | 1.327 (2)   | O2—C14  | 1.421 (3) |
| C7—C8  | 1.464 (2)   | C14—O3  | 1.433 (2) |
| C8—C13 | 1.392 (2)   |         |           |

Almost all H atoms were located in difference Fourier maps but they were eventually placed in calculated positions ( $C-H = 0.93-0.98 \text{ \AA}$ ) and refined in the riding-model approximation with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C,N})$ , or  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$  for methyl C atoms.

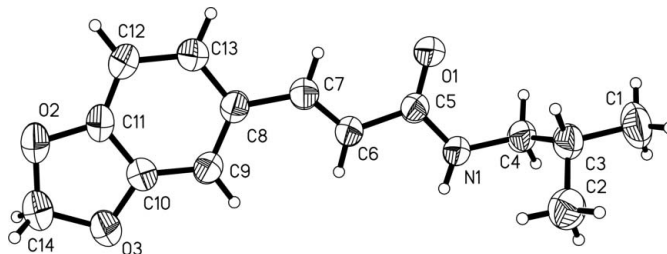


Figure 1

The molecular structure of (I) with displacement ellipsoids drawn at the 45% probability level and H atoms as small spheres.

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Siemens, 1996); software used to prepare material for publication: SHELXTL.

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