2-Phenyl-8,9,10,11-tetrahydro-1-benzothieno[3,2-e][1,2,4]triazolo[1,5-c]pyrimidine

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In the title compound, C₁₅H₁₂N₆S, the benzothieno moiety is fused at one end of the pyrimidine ring while the triazole ring with a phenyl substituent is fused at the other side. The triazole ring is almost planar [maximum deviation = 0.0028 (3) Å] while the cyclohexane ring adopts a half-chair conformation. In the crystal, pairs of intermolecular C–H···N hydrogen bonds form centrosymmetric head-to-head dimers, corresponding to an R(8) graph-set motif. Further C–H···N interactions generate a zigzag chain of molecules along the c axis. The supramolecular assembly is consolidated by π–π stacking interactions [centroid–centroid distance = 3.44Å (4) Å].

Related literature

For the biological activity of thiophenes, benzenothiophenes, pyrimidines and triazolopyrimidines, see: Shishoo & Jain (1992); Bradbury & Rivett (1991); Elslager et al. (1981); Yunosov et al. (1966); Blain et al. (1982). For related structures, see: Akkurt et al. (2008); Buzylkin et al. (2008); Harrison et al. (2006); Lipson et al. (2006); Belcher & Squatrito (2006). For hydrogen-bond motifs, see: Bernstein et al. (1995). For puckering and asymmetry parameters, see: Cremer & Pople (1975); Nardelli (1983).

Table 1

Hydrogen-bond geometry (Å, °).

<table>
<thead>
<tr>
<th>D···H···A</th>
<th>D···H</th>
<th>H···A</th>
<th>D···A</th>
<th>D···A</th>
</tr>
</thead>
<tbody>
<tr>
<td>C=S–H···N2⁺</td>
<td>0.93</td>
<td>2.50</td>
<td>3.413 (3)</td>
<td>166</td>
</tr>
<tr>
<td>C11–H11B···–N2⁺</td>
<td>0.97</td>
<td>2.82</td>
<td>3.653 (5)</td>
<td>144</td>
</tr>
</tbody>
</table>

Symmetry codes: (i) −x−1, −y+1, −z; (ii) x, −y+1, −z+1.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT-Plus (Bruker, 1998); data reduction: SAINT-Plus; program(s) used to solve structure: SHELX97 (Sheldrick, 2008); program(s) used to refine structure: SHEXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 (Farrugia, 1997) and CAMERON (Watkin et al., 1996); software used to prepare material for publication: WinGX (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PB056).

References
