

2-(4-Hydroxy-2-oxo-2,3-dihydro-1,3-benzothiazol-7-yl)-ethyl-ammonium chloride

Experimental

| | |
|---------------------|---|
| Chemical Formula | C ₉ H ₁₁ N ₂ O ₂ S . Cl |
| Sample presentation | 0.7 mm borosilicate glass capillary |
| Diffractometer | Bruker AXS D8 Advance $\theta/2\theta$, 2 kW |
| Monochromator | Primary focusing, Ge 111, $2\theta_{\text{mono}} = 26^\circ$ |
| Geometry | Transmission |
| λ | CuK α_1 , 1.54056 Å |
| Detector | PSD system Braun OED-50M |
| Temperature / K | 293 |

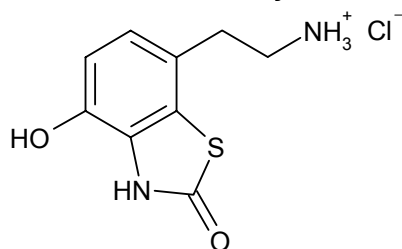
Diffraction data

| | |
|------------------------------------|-------------|
| Filename | pd_0014.xye |
| Data range / $^\circ 2\theta$ | 5-61 |
| Step size / $^\circ 2\theta$ | 0.0145 |
| Count time / seconds | 10 |
| Total data collection time / hours | ca.10 |

Crystallography

| | | | |
|--|----------|--------|--------|
| Space group | $P2_1/a$ | | |
| Approximate lattice parameters / Å, $^\circ$ | 7.555 | 14.640 | 10.246 |
| | 90 | 109.30 | 90 |

Connectivity



Citation

Use of the Data should acknowledge the following citation:

A.J. Florence, N. Shankland, K. Shankland, W.I.F. David, E. Pidcock, X. Xu, A. Johnston, A.R. Kennedy, P.J. Cox, J.S.O. Evans, G. Steele, S.D. Cosgrove & C.S. Frampton (2005). Solving molecular crystal structures from laboratory X-ray powder diffraction data with DASH: the state of the art and challenges, *Journal of Applied Crystallography*, 38, 249-259.

Acknowledgement

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Other information