

# Thianaphthene-3-acetonitrile

|                      |                                                                                                       |
|----------------------|-------------------------------------------------------------------------------------------------------|
| Other names:         | Benzo[b]thiophene-3-acetonitrile<br>Acetonitrile, 2-(3-benzothiény)-<br>1-Benzothien-3-ylacetonitrile |
| Inchi:               | InChI=1S/C10H7NS/c11-6-5-8-7-12-10-4-2-1-3-9(8)10/h1-4,7H,5H2                                         |
| InchiKey:            | DEELHLMCCWZFFE-UHFFFAOYSA-N                                                                           |
| Formula:             | C10H7NS                                                                                               |
| SMILES:              | N#CCc1csc2ccccc12                                                                                     |
| Mol. weight [g/mol]: | 173.24                                                                                                |

## Physical Properties

| Property code | Value   | Unit   | Source             |
|---------------|---------|--------|--------------------|
| logp          | 2.967   |        | Crippen Method     |
| mcvol         | 130.570 | ml/mol | McGowan Method     |
| tb            | 594.50  | K      | Cheméo Relay (1.0) |

## Sources

|                           |                                                                                                                                             |
|---------------------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| Crippen Method:           | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                   |
| Crippen Method:           | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                           |
| Cheméo Relay (1.0):       |                                                                                                                                             |
| Cheméo Relay (1.0, beta): |                                                                                                                                             |
| NIST Webbook:             | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C3216486&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3216486&amp;Units=SI</a> |
| McGowan Method:           | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                       |

## Legend

|        |                                     |
|--------|-------------------------------------|
| logp:  | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume     |
| tb:    | Normal Boiling Point Temperature    |

Latest version available from:

<https://www.chemeo.com/cid/11-136-8/Thianaphthene-3-acetonitrile.pdf>

Generated by Cheméo on 2026-07-21 20:59:37.608764144 +0000 UTC m=+178673.450649578.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.