

# 2-PROPYLTHIAZOLE

|                      |                                                    |
|----------------------|----------------------------------------------------|
| Other names:         | 2-n-Propylthiazole<br>Thiazole, 2-propyl-          |
| Inchi:               | InChI=1S/C6H9NS/c1-2-3-6-7-4-5-8-6/h4-5H,2-3H2,1H3 |
| InchiKey:            | CMOIEFFAOUQJPS-UHFFFAOYSA-N                        |
| Formula:             | C6H9NS                                             |
| SMILES:              | CCCC1NCCS1                                         |
| Mol. weight [g/mol]: | 127.21                                             |

## Physical Properties

| Property code | Value   | Unit   | Source             |
|---------------|---------|--------|--------------------|
| logp          | 2.096   |        | Crippen Method     |
| mcvol         | 102.270 | ml/mol | McGowan Method     |
| rinpol        | 981.00  |        | NIST Webbook       |
| rinpol        | 969.00  |        | NIST Webbook       |
| ripol         | 1372.00 |        | NIST Webbook       |
| ripol         | 1381.00 |        | NIST Webbook       |
| tb            | 437.62  | K      | Cheméo Relay (1.0) |
| tf            | 205.91  | K      | Cheméo Relay (1.0) |

## Sources

|                           |                                                                                                                                               |
|---------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| NIST Webbook:             | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C17626754&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C17626754&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>                         |
| Crippen Method:           | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>                                     |
| Crippen Method:           | <a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>                             |
| Cheméo Relay (1.0):       |                                                                                                                                               |
| Cheméo Relay (1.0, beta): |                                                                                                                                               |

## Legend

|       |                                     |
|-------|-------------------------------------|
| logp: | Octanol/Water partition coefficient |
|-------|-------------------------------------|

|                |                                  |
|----------------|----------------------------------|
| <b>mcvol:</b>  | McGowan's characteristic volume  |
| <b>rinpol:</b> | Non-polar retention indices      |
| <b>ripol:</b>  | Polar retention indices          |
| <b>tb:</b>     | Normal Boiling Point Temperature |
| <b>tf:</b>     | Normal melting (fusion) point    |

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