

# 5-Nitrothiophene-2-carboxaldehyde

|                      |                                                                                                                                                                                       |
|----------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | 2-Thiophenecarboxaldehyde, 5-nitro-<br>5-Nitro 2-thiophenecarboxaldehyde<br>5-Nitrothiophene-2-carboxaldehyde<br>5-nitrothiophene-2-carbaldehyde<br>Thiophenecarboxaldehyde, 5-nitro- |
| Inchi:               | InChI=1S/C5H3NO3S/c7-3-4-1-2-5(10-4)6(8)9/h1-3H                                                                                                                                       |
| InchiKey:            | CHTSWZNXEKOLPM-UHFFFAOYSA-N                                                                                                                                                           |
| Formula:             | C5H3NO3S                                                                                                                                                                              |
| SMILES:              | O=Cc1ccc([N+](=O)[O-])s1                                                                                                                                                              |
| Mol. weight [g/mol]: | 157.15                                                                                                                                                                                |

## Physical Properties

| Property code | Value  | Unit   | Source             |
|---------------|--------|--------|--------------------|
| hvap          | 72.06  | kJ/mol | Cheméo Relay (1.0) |
| logp          | 1.469  |        | Crippen Method     |
| mcvol         | 97.190 | ml/mol | McGowan Method     |
| tf            | 350.82 | 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=C4521339&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4521339&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

|       |                                                 |
|-------|-------------------------------------------------|
| hvap: | Enthalpy of vaporization at standard conditions |
| logp: | Octanol/Water partition coefficient             |

**mcvol:** McGowan's characteristic volume  
**tf:** Normal melting (fusion) point

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