

2-Nitrothiophene-4-carbonitrile

Inchi: InChI=1S/C5H2N2O2S/c6-2-4-1-5(7(8)9)10-3-4/h1,3H
InchiKey: NACMZLGGHMPMKQ-UHFFFAOYSA-N
Formula: C5H2N2O2S
SMILES: N#Cc1csc([N+](=O)[O-])c1
Mol. weight [g/mol]: 154.15
CAS: 42137-24-6

Physical Properties

| Property code | Value | Unit | Source |
|---------------|--------|--------|----------------|
| log10ws | -2.23 | | Crippen Method |
| logp | 1.528 | | Crippen Method |
| mcvol | 97.000 | ml/mol | McGowan Method |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C42137246&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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