

2-methyl-5,7-dihydrothieno[3,4-d]pyrimidine

Inchi: InChI=1S/C7H8N2S/c1-5-8-2-6-3-10-4-7(6)9-5/h2H,3-4H2,1H3
InchiKey: XSUYIZJJKIKWFN-UHFFFAOYSA-N
Formula: C7H8N2S
SMILES: Cc1ncc2c(n1)CSC2
Mol. weight [g/mol]: 152.22

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -3.02 | | Crippen Method |
| logp | 1.532 | | Crippen Method |
| mcvol | 111.180 | ml/mol | McGowan Method |
| rinpol | 1339.00 | | NIST Webbook |
| rinpol | 1339.00 | | NIST Webbook |
| ripol | 2137.00 | | NIST Webbook |

Sources

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=R169254&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
ripol: Polar retention indices

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