

Thiantoin

Inchi: InChI=1S/C13H10N2O2S/c16-11-13(15-12(17)14-11,10-7-4-8-18-10)9-5-2-1-3-6-9/h1-8H
InchiKey: DCPACFSINCUFEC-UHFFFAOYSA-N
Formula: C13H10N2O2S
SMILES: O=C1NC(=O)C(c2ccccc2)(c2cccs2)N1
Mol. weight [g/mol]: 258.30
CAS: 7772-37-4

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -3.14 | | Crippen Method |
| logp | 1.831 | | Crippen Method |
| mcvol | 179.400 | ml/mol | McGowan Method |
| rinpol | 2145.00 | | NIST Webbook |
| rinpol | 2145.00 | | NIST Webbook |

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C7772374&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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<https://www.chemeo.com/cid/121-939-5/Thiantoin.pdf>

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