

# 1-Ethyltheobromine

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C9H12N4O2/c1-4-13-8(14)6-7(10-5-11(6)2)12(3)9(13)15/h5H,4H2,1-3H3 |
| <b>InchiKey:</b>            | KRVVZXPQPXJE-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C9H12N4O2  |
| <b>SMILES:</b>              | CCn1c(=O)c2c(ncn2C)n(C)c1=O  |
| <b>Mol. weight [g/mol]:</b> | 208.22   |

## Physical Properties

| Property code | Value   | Unit   | Source  |
|---------------|---------|--------|---|
| log10ws       | -0.72   |        | Aqueous and cosolvent solubility data for drug-like organic compounds |
| logp          | -0.546  |        | Crippen Method  |
| mcvol         | 150.410 | ml/mol | McGowan Method  |

## Sources

|   |   |
|---|---|
| <b>Crippen Method:</b>  | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                 |
| <b>Aqueous and cosolvent solubility data for drug-like organic compounds:</b> | <a href="https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/">https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/</a> |
| <b>McGowan Method:</b>  | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>     |

## Legend

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

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