# 1-Ethyltheobromine

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

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Aqueous and cosolvent solubility data for drug-like organic compounds:** https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

## Legend

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