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