1-Butyltheobromine

Inchi: InChI=1S/C11H16N4O2/c1-4-5-6-15-10(16)8-9(12-7-13(8)2)14(3)11(15)17/h7H,4-6H2,1-
InchiKey: ZCUPBJOZMPROIJ-UHFFFAOYSA-N
Formula: C11H16N4O2
SMILES: CCCCn1c(=O)c2c(ncn2C)n(C)c1=O
Mol. weight [g/mol]: 236.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.62		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	0.234		Crippen Method
mcvol	178.590	ml/mol	McGowan Method

Sources

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
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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