Isbufylline

Inchi: InChI=1S/C11H16N4O2/c1-7(2)5-15-6-12-9-8(15)10(16)14(4)11(17)13(9)3/h6-7H,5H2,1-
InchiKey: WHUWQSQEVISUMC-UHFFFAOYSA-N
Formula: C11H16N4O2
SMILES: CC(C)Cn1cnc2c1c(=O)n(C)c(=O)n2C
Mol. weight [g/mol]: 236.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.94		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	0.090		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