7-butyl-1,3,8-trimethylpurine-2,6-dione

Inchi: InChI=1S/C12H18N4O2/c1-5-6-7-16-8(2)13-10-9(16)11(17)15(4)12(18)14(10)3/h5-7H2,1
InchiKey: WCXBUFRTRWDHOX-UHFFFAOYSA-N
Formula: C12H18N4O2
SMILES: CCCCn1c(C)nc2c1c(=O)n(C)c(=O)n2C
Mol. weight [g/mol]: 250.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.75		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	0.542		Crippen Method
mcvol	192.680	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
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/

Legend

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