1,3,8-trimethyl-7-(2-methylpropyl)purine-2,6-dione

Inchi: InChI=1S/C12H18N4O2/c1-7(2)6-16-8(3)13-10-9(16)11(17)15(5)12(18)14(10)4/h7H,6H2
InchiKey: VUYNLAZRVSUFDB-UHFFFAOYSA-N
Formula: C12H18N4O2
SMILES: Cc1nc2c(c(=O)n(C)c(=O)n2C)n1CC(C)C
Mol. weight [g/mol]: 250.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.60		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	0.398		Crippen Method
mcvol	192.680	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