



Formula: C₈H₁₀N₄O₂

MW: 194.19

CAS: 58-08-2

MDL: MFCD00005758

TNP: TNP00310

METHYLTHEOBROMIDE; METHYLTHEOBROMINE; CAFFEIN; CAFFEINE; COFFEIN;
COFFEINE; COFFEINUM; GUARANINE



LogP: 1.16

LogS: -5.51

Acceptors: 2

Donors: 0

Rotation Bonds: 0

Chiral Centers: 0

N+O: 6

LIPINSKY: 4

IUPAC: 1,3,7-trimethyl-1,3,7-trihydropurine-2,6-dione

Smiles: c12c(c(=O)n(c(n1C)=O)C)n(C)cn2

Specification: Purine; Alkaloids; Alkaloids (Others); Biochemistry; Intermediates & Fine
Chemicals; Pharmaceuticals; Food & Flavor Additives; Cyclic Nucleotide related; Signalling
Caffeine Chemical Properties:

mp 234-236.5 C(lit.) bp 178C density 1.23 FEMA 2224 Fp 178C storage temp. 2-8C Water
Solubility 20 g/L (20