



Formula: C₇H₈N₄O₂

MW: 180.17

CAS: 83-67-0

TNP NUMBER: TNP00408

MDL NUMBER: MFCD00022830

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

Smiles: n1c2c(c([nH]c(n2C)=O)=O)n(c1)C

Theobromine 99%

THERAPEUTIC CATEGORY: Diuretic, broncholidator, cardi tonic

VET THERAP CATEGORY: Diuretic, myocardial stimulant, vasodilator

REFERENCE: Merck 12, 9418

SOURCE: The principle alkaloid of the cacao bean

ACCEPTORS: 2

DONORS: 1

ROTATION BONDS: 0

N+O: 6

Chiral Centers: 0

LogP: -0.67

LogS: -2.49

LIPINSKI: 4

Synonyms:

3,7-dihydro-3,7-dimethyl-1h-purine-6-dione;3,7-Dimethyl-3,7-dihydro-1H-purine-2,6-dione;3,7-dimethyl-xanthin;6-dione,3,7-dihydro-3,7-dimethyl-1H-Purine-2;Diurobromine;Santheose;SC 15090;sc15090

CAS:83-67-0

MF:C7H8N4O2

MW:180.16

EINECS:201-494-2

Product Categories:Heterocyclic Compounds;Alkaloids;Alkaloids (Others);Biochemistry;Heterocycles;Intermediates & Fine Chemicals;Metabolites & Impurities;Pharmaceuticals Theobromine

Chemical Properties: mp 345-350 C density 1.50 FEMA 3591 Fp 290-295C solubility H2O: slightly soluble form solid color white Water Solubility slightly soluble,