

Theobromine

Other names:	1H-Purine-2,6-dione, 3,7-dihydro-3,7-dimethyl- 3,7-Dimethylxanthine 3,7-dimethyl-3,7-dihydro-1H-purine-2,6-dione Diurobromine NSC 5039 SC 15090 Santheose Teobromin Theosalvose Theostene Thesal Thesodate Xanthine, 3,7-dimethyl-
Inchi:	InChI=1S/C7H8N4O2/c1-10-3-8-5-4(10)6(12)9-7(13)11(5)2/h3H,1-2H3,(H,9,12,13)
InchiKey:	YAPQBXQYLJRXSA-UHFFFAOYSA-N
Formula:	C7H8N4O2
SMILES:	Cn1cnc2c1c(=O)[nH]c(=O)n2C
Mol. weight [g/mol]:	180.16
CAS:	83-67-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.59		Aqueous Solubility Prediction Method
log10ws	-2.52		Estimated Solubility Method
logp	-1.522		Crippen Method
mcvol	122.230	ml/mol	McGowan Method
tf	627.90	K	Aqueous Solubility Prediction Method

Sources

Equilibrium partitioning of drug molecules between aqueous and amino acid ester-based ionic liquids:	https://www.doi.org/10.1016/j.jct.2013.02.011
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Volumetric, Viscometric and Spectroscopic Approach to Study the Solvation Behavior of Xanthine Drugs in Aqueous Solutions of NaCl at T = 288.15-318.15 K and at p = 101.325 kPa: Studies on Caffeine, Theophylline, and Theophylline in Aqueous Solutions and in Organic Solvents at 288.15 K and at Pressure p = 101.3 kPa:
Crippen Method:

Aqueous Solubility Prediction Method:

Measurement and Correlation of Solubility of Theobromine, Theophylline, and Caffeine in Water and Organic Solvents at Various Temperatures:

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point

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<https://www.doi.org/10.1021/acs.jced.6b00273>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C83670&Units=SI>

<https://www.doi.org/10.1021/acs.jced.7b00520>

<https://www.doi.org/10.1016/j.jct.2014.05.005>

<http://link.springer.com/article/10.1007/BF02311772>

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

<https://www.doi.org/10.1021/acs.jced.7b00065>