

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 media and their physical chemical properties and solubility of pharmaceuticals - Methyl xanthines:	https://www.doi.org/10.1016/j.jct.2013.02.011
	https://www.doi.org/10.1016/j.jct.2014.05.005

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Measurement and Correlation of Solubility of Theobromine, Caffeine, and Theophylline in Water and Organic Solvents at Various Temperatures: Estimated Solubility Method:	https://www.doi.org/10.1021/acs.jced.7b00065
NIST Webbook:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Volumetric, Viscometric and Spectroscopic Approach to Study the Solvation Behavior of Kainine and Theobromine Drugs in Aqueous Solutions of NaCl, LiCl, and CsCl: Solubility in Aqueous Solvents:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
MgCl₂ at Temperatures T = (288.15 to 318.15) K and at Pressure p = 101.3 kPa:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C83670&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/68-142-9/Theobromine.pdf>

Generated by Cheméo on 2024-04-10 04:02:14.957189313 +0000 UTC m=+15010983.877766637.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.