Theophylline

Other names:	1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-, monohydrate
	1H-Purine-2,6-dione, 3,9-dihydro-1,3-dimethyl-, hydrate (1:1)
	theophylline monohydrate
Inchi:	InChI=1S/C7H8N4O2.H2O/c1-10-5-4(8-3-9-5)6(12)11(2)7(10)13;/h3H,1-2H3,(H,8,9);1H2
InchiKey:	INQSMEFCAIHTJG-UHFFFAOYSA-N
Formula:	C7H10N4O3
SMILES:	Cn1c(=O)c2[nH]cnc2n(C)c1=O.O
Mol. weight [g/mol]:	198.18
CAS:	5967-84-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.32		Aqueous Solubility Prediction Method
log10ws	-1.39		Estimated Solubility Method
tf	544.98	K	Aqueous Solubility Prediction Method

Sources

Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5967840&Units=SI
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

log10ws:	Log10 of Water solubility in mol/l
tf:	Normal melting (fusion) point