1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-7-[2-[(1-methyl-2-phenyle

Other names: Fenethylline
7-[2-[(«alpha»-Methylphenethyl)amino]methyl]theophylline
Theophyllineethylamphetamine
Theophylline, 7-(2-((alpha-methylphenethyl)amino)ethyl)-

Inchi: InChI=1S/C18H23N5O2/c1-13(11-14-7-5-4-6-8-14)19-9-10-23-12-20-16-15(23)17(24)22(

InchiKey: NMCHYWGKBADVMK-UHFFFAOYSA-N

Formula: C18H23N5O2

SMILES: CC(Cc1ccccc1)NCCn1cnc2c1c(=O)n(C)c(=O)n2C

Mol. weight [g/mol]: 341.41

CAS: 3736-08-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.90		Crippen Method
logp	0.654		Crippen Method
mcvol	263.440	ml/mol	McGowan Method
rinpol	2820.00		NIST Webbook
rinpol	2830.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3736081&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices