

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

Other names:	Fenethylamine 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/ci990307I

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

rinpol: Non-polar retention indices

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