1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-8-(phenylmethyl)-

Other names: 8-Benzyltheophylline
8-benzyl-3,7-dihydro-1,3-dimethyl-1H-purine-2,6-dione
8-(phenylmethyl)theophylline

Inchi: InChI=1S/C14H14N4O2/c1-17-12-11(13(19)18(2)14(17)20)15-10(16-12)8-9-6-4-3-5-7-9/h

InchiKey: SWKGFZTXWQMFLK-UHFFFAOYSA-N

Formula: C14H14N4O2

SMILES: Cn1c(=O)c2[nH]c(Cc3ccccc3)nc2n(C)c1=O

Mol. weight [g/mol]: 270.29

CAS: 2879-15-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.78		Crippen Method
logp	0.069		Crippen Method
mcvol	197.100	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2879154&Units=SI

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

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

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume