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

Other names: Theophylline, 8-(hydroxymethyl)-
1H-purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-8phenylmethyl)-
Inchi: InChI=1S/C8H10N4O3/c1-11-6-5(9-4(3-13)10-6)7(14)12(2)8(11)15/h13H,3H2,1-2H3,(H,9
InchiKey: GHYKZCOUOKEWNN-UHFFFAOYSA-N
Formula: C8H10N4O3
SMILES: Cn1c(=O)c2[nH]c(CO)nc2n(C)c1=O
Mol. weight [g/mol]: 210.19
CAS: 2879-16-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.82		Crippen Method
logp	-2.029		Crippen Method
mcvol	142.190	ml/mol	McGowan Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2879165&Units=SI

Legend

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

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