4,5,6,7-Tetrahydropyrazolo[1,5-d][1,2,4]-triazin-4-one-2,6,7,7-tetramethyl

Inchi: InChI=1S/C9H16N4O/c1-6-5-7-8(14)11-12(4)9(2,3)13(7)10-6/h7H,5H2,1-4H3,(H,11,14)

InchiKey: WPBAKWWCBWRZED-UHFFFAOYSA-N

Formula: C9H16N4O

SMILES: CC1=NN2C(C1)C(O)=NN(C)C2(C)C

Mol. weight [g/mol]: 196.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.37		Crippen Method
logp	0.990		Crippen Method
mcvol	153.140	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R582340&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