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

Inchi: InChI=1S/C8H14N4O/c1-6-4-7-8(13)11(3)10(2)5-12(7)9-6/h7H,4-5H2,1-3H3

InchiKey: NORATMVMRQWQBX-UHFFFAOYSA-N

Formula: C8H14N4O

SMILES: CC1=NN2CN(C)N(C)C(=O)C2C1

Mol. weight [g/mol]: 182.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.20		Crippen Method
logp	-0.287		Crippen Method
mcvol	139.050	ml/mol	McGowan Method
rinpol	1939.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R582246&Units=SI

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

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices