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

Inchi: InChI=1S/C11H20N4O/c1-4-5-6-15-11(16)10-7-9(2)12-14(10)8-13(15)3/h10H,4-8H2,1-3H

InchiKey: BFBPOHRWWMHBJN-UHFFFAOYSA-N

Formula: C11H20N4O

SMILES: CCCCN1C(=O)C2CC(C)=NN2CN1C

Mol. weight [g/mol]: 224.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.45		Crippen Method
logp	0.883		Crippen Method
mcvol	181.320	ml/mol	McGowan Method
rinpol	2160.00		NIST Webbook

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=R582286&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices