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

Inchi: InChI=1S/C10H18N4O/c1-4-5-14-10(15)9-6-8(2)11-13(9)7-12(14)3/h9H,4-7H2,1-3H3

InchiKey: SVUOBZNKEQSVHJ-UHFFFAOYSA-N

Formula: C10H18N4O

SMILES: CCCN1C(=O)C2CC(C)=NN2CN1C

Mol. weight [g/mol]: 210.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.03		Crippen Method
logp	0.493		Crippen Method
mcvol	167.230	ml/mol	McGowan Method
rinpol	2070.00		NIST Webbook

Sources

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=R582335&Units=SI

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices