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

Inchi: InChI=1S/C9H16N4O/c1-4-13-9(14)8-5-7(2)10-12(8)6-11(13)3/h8H,4-6H2,1-3H3
InchiKey: UMJPLVHCKVBHMN-UHFFFAOYSA-N
Formula: C9H16N4O
SMILES: CCN1C(=O)C2CC(C)=NN2CN1C
Mol. weight [g/mol]: 196.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.62		Crippen Method
logp	0.103		Crippen Method
mcvol	153.140	ml/mol	McGowan Method
rinpol	2006.00		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=R582291&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