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

Inchi: InChI=1S/C11H18N4O/c1-8-7-9-10(16)14(2)13-11(15(9)12-8)5-3-4-6-11/h9,13H,3-7H2,1

InchiKey: UURHHYSBRAMJBX-UHFFFAOYSA-N

Formula: C11H18N4O

SMILES: CC1=NN2C(C1)C(=O)N(C)NC21CCCC1

Mol. weight [g/mol]: 222.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.08		Crippen Method
logp	0.684		Crippen Method
mcvol	170.460	ml/mol	McGowan Method
rinpol	1842.00		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=R582320&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