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

Inchi: InChI=1S/C12H20N4O/c1-9-8-10-11(17)14-15(2)12(16(10)13-9)6-4-3-5-7-12/h10H,3-8H2
InchiKey: MOZSDTSHKOXRJU-UHFFFAOYSA-N
Formula: C12H20N4O
SMILES: CC1=NN2C(C1)C(=O)NN(C)C21CCCCC1
Mol. weight [g/mol]: 236.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.50		Crippen Method
logp	1.074		Crippen Method
mcvol	184.550	ml/mol	McGowan Method
rinpol	1983.00		NIST Webbook
rinpol	1983.00		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=R582360&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

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