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

Inchi: InChI=1S/C12H20N4O/c1-9-8-10-11(17)15(2)14-12(16(10)13-9)6-4-3-5-7-12/h10,14H,3-8

InchiKey: KBTUGDJZPHLIKC-UHFFFAOYSA-N

Formula: C12H20N4O

SMILES: CC1=NN2C(C1)C(=O)N(C)NC21CCCCC1

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	1955.00		NIST Webbook
rinpol	1955.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R582315&Units=SI

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.