Pyrazolo[1,5-d][1,2,4]triazin-3-one, 2,5,6-trimethyl-7,7-pentamethylene

Inchi: InChI=1S/C13H20N4O/c1-10-12(18)11-9-15(2)16(3)13(17(11)14-10)7-5-4-6-8-13/h9H,4-

InchiKey: SYTRPDHLUDZPMR-UHFFFAOYSA-N

Formula: C13H20N4O

SMILES: CC1=NN2C(=CN(C)N(C)C23CCCCC3)C1=O

Mol. weight [g/mol]: 248.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.53		Crippen Method
logp	1.541		Crippen Method
mcvol	194.340	ml/mol	McGowan Method
rinpol	1939.00		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=R154633&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