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

Inchi: InChI=1S/C12H18N4O/c1-9-11(17)10-8-13-15(2)12(16(10)14-9)6-4-3-5-7-12/h8,13H,3-7

InchiKey: HMGCVNUSYNMQSH-UHFFFAOYSA-N

Formula: C12H18N4O

SMILES: CC1=NN2C(=CNN(C)C23CCCCC3)C1=O

Mol. weight [g/mol]: 234.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.73		Crippen Method
logp	1.199		Crippen Method
mcvol	180.250	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=R154673&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

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