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

Inchi: InChI=1S/C11H16N4O/c1-8-7-9-10(16)13-14(2)11(15(9)12-8)5-3-4-6-11/h7H,3-6H2,1-2H

InchiKey: PPICRJRHTGFGJA-UHFFFAOYSA-N

Formula: C11H16N4O

SMILES: Cc1cc2n(n1)C1(CCCC1)N(C)NC2=O

Mol. weight [g/mol]: 220.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.09		Crippen Method
logp	1.009		Crippen Method
mcvol	166.160	ml/mol	McGowan Method
rinpol	1853.00		NIST Webbook
rinpol	1853.00		NIST Webbook

Sources

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=R154688&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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.