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

Inchi: InChI=1S/C13H14N4O/c1-9-8-11-12(18)15-16(2)13(17(11)14-9)10-6-4-3-5-7-10/h3-8,13H

InchiKey: RUFNUJIQQGZOLS-UHFFFAOYSA-N

Formula: C13H14N4O

SMILES: Cc1cc2n(n1)C(c1ccccc1)N(C)NC2=O

Mol. weight [g/mol]: 242.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.53		Crippen Method
logp	1.329		Crippen Method
mcvol	181.440	ml/mol	McGowan Method
rinpol	2047.00		NIST Webbook
rinpol	2047.00		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=R154693&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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