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

Inchi: InChI=1S/C9H14N4O/c1-6-5-7-8(14)11-12(4)9(2,3)13(7)10-6/h5H,1-4H3,(H,11,14)
InchiKey: BEVVZHLXOHZILQ-UHFFFAOYSA-N
Formula: C9H14N4O
SMILES: Cc1cc2n(n1)C(C)(C)N(C)NC2=O
Mol. weight [g/mol]: 194.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.36		Crippen Method
logp	0.474		Crippen Method
mcvol	148.840	ml/mol	McGowan Method
rinpol	1600.00		NIST Webbook
rinpol	1600.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R154668&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.