4,5,6,7-Tetrahydropyrazolo[1,5-d][1,2,4]-triazin-4-one-2,5,6,7,7-pentamethyl

Inchi: InChI=1S/C10H18N4O/c1-7-6-8-9(15)12(4)13(5)10(2,3)14(8)11-7/h8H,6H2,1-5H3
InchiKey: BPQWYIMOBBMGIV-UHFFFAOYSA-N
Formula: C10H18N4O
SMILES: CC1=NN2C(C1)C(=O)N(C)N(C)C2(C)C
Mol. weight [g/mol]: 210.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.15		Crippen Method
logp	0.491		Crippen Method
mcvol	167.230	ml/mol	McGowan Method
rinpol	1552.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R582231&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices