

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

InChI: C12H20N4O/c1-9-8-10-11-17)1-(2)15(3)12(16(10)13-9)6-4-5-7-12/h10H,4-8H2
InChIKey: UYZPWZQYXITPBC-UHFFFAOYSA-N
Formula: C12H20N4O
SMILES: CC1=NN2C(C1)C(=O)N(C)N(C)C21CCCC1
Mol. weight [g/mol]: 236.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.88		Crippen Method
logp	1.026		Crippen Method
mcvol	184.550	ml/mol	McGowan Method
rinpol	1807.00		NIST Webbook
rinpol	1807.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R582266&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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