

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

InChI: CN1C=NN2C(C1)C(=O)N(C)NC2(C)C
InChIKey: BKNRLKWNMLJXSH-UHFFFAOYSA-N

Formula: C₉H₁₆N₄O
SMILES: CC1=NN2C(C1)C(=O)N(C)NC2(C)C
Mol. weight [g/mol]: 196.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.35		Crippen Method
logp	0.149		Crippen Method
mcvol	153.140	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R582271&Units=SI>
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>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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