

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

InChI: CN1C=NC2C(C1)C(=O)N(C)N(C)C2(C)C
InChIKey: BPQWYIMOBMMGV-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/ci990307I
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

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