

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

InChI: Cc1=nc2c(c1)nc(=O)c2C

InChIKey: KCIXKZQUQZKZJP-UHFFFAOYSA-N

Formula: C7H12N4O

SMILES: CC1=NN2CNN(C)C(=O)C2C1

Mol. weight [g/mol]: 168.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.40		Crippen Method
logp	-0.629		Crippen Method
mcvol	124.960	ml/mol	McGowan Method
rinpole	1600.00		NIST Webbook

Sources

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=R582300&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

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

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