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

Inchi: InChI=1S/C7H12N4O/c1-5-3-6-7(12)10(2)8-4-11(6)9-5/h6,8H,3-4H2,1-2H3
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
rinpol	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
rinpol: Non-polar retention indices