3-Amino-5,6-dimethyltriazolo[4,3-a]pyrazine

Inchi: InChI=1S/C7H9N5/c1-4-5(2)12-6(3-9-4)10-11-7(12)8/h3H,1-2H3,(H2,8,11)
InchiKey: GDYUNQBKJKHPBK-UHFFFAOYSA-N
Formula: C7H9N5
SMILES: Cc1ncc2nnc(N)n2c1C
Mol. weight [g/mol]: 163.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.31		Crippen Method
logp	0.323		Crippen Method
mcvol	120.470	ml/mol	McGowan Method
rinpol	1758.00		NIST Webbook
rinpol	1758.00		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=R74800&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.