1H-pyrazolo[3,4-d]pyrimidine, 4-amino-1-methyl-

Inchi: InChI=1S/C6H7N5/c1-11-6-4(2-10-11)5(7)8-3-9-6/h2-3H,1H3,(H2,7,8,9)
InchiKey: JBMTUXVKTGBMLE-UHFFFAOYSA-N
Formula: C6H7N5
SMILES: Cn1ncc2c(N)ncnc21
Mol. weight [g/mol]: 149.15
CAS: 5334-99-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.49		Crippen Method
logp	-0.054		Crippen Method
mcvol	106.380	ml/mol	McGowan Method

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=C5334996&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