1,3,5-Trimethyl-1H-pyrazol-4-amine

Other names: 4-Amino-1,3,5-trimethylpyrazole
Inchi: InChI=1S/C6H11N3/c1-4-6(7)5(2)9(3)8-4/h7H2,1-3H3
InchiKey: SSDGMKHZMNTWLS-UHFFFAOYSA-N
Formula: C6H11N3
SMILES: Cc1nn(C)c(C)c1N
Mol. weight [g/mol]: 125.17
CAS: 28466-21-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.11		Crippen Method
logp	0.619		Crippen Method
mcvol	105.880	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C28466219&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume