3(4)-methylpyrrolo(1,2-a)pyrazine

Inchi: InChI=1S/C8H8N2/c1-7-5-9-8-3-2-4-10(8)6-7/h2-6H,1H3
InchiKey: ZOOIAHZREFDCEN-UHFFFAOYSA-N
Formula: C8H8N2
SMILES: Cc1cnc2cccn2c1
Mol. weight [g/mol]: 132.16

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.67		Crippen Method
logp	1.643		Crippen Method
mcvol	104.620	ml/mol	McGowan Method
rinpol	1317.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R230430&Units=SI

Legend

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