1H-Pyrrole, 2,3-dimethyl-

Other names: 2,3-dimethyl-1H-pyrrole
Inchi: InChI=1S/C6H9N/c1-5-3-4-7-6(5)2/h3-4,7H,1-2H3
InchiKey: OUYLXVQKVBXUGW-UHFFFAOYSA-N
Formula: C6H9N
SMILES: Cc1cc[nH]c1C
Mol. weight [g/mol]: 95.14
CAS: 600-28-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.64		Crippen Method
logp	1.150		Crippen Method
mcvol	85.920	ml/mol	McGowan Method
rinpol	804.00		NIST Webbook
ripol	1620.00		NIST Webbook
ripol	1620.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C600282&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
rinpol: Non-polar retention indices
ripol: Polar retention indices