N-(2,5-Dimethylpyrrol-L-yl)formamide

Inchi: InChI=1S/C7H10N2O/c1-6-3-4-7(2)9(6)8-5-10/h3-5H,1-2H3,(H,8,10)
InchiKey: JKTLFKQRLWMPSQ-UHFFFAOYSA-N
Formula: C7H10N2O
SMILES: Cc1ccc(C)n1NC=O
Mol. weight [g/mol]: 138.17
CAS: 143800-06-0

Physical Properties

Property code	Value	Unit	Source
ie	7.88	eV	NIST Webbook
log10ws	-1.66		Crippen Method
logp	0.805		Crippen Method
mcvol	111.560	ml/mol	McGowan Method

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=C143800060&Units=SI

Legend

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

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