1H-Pyrrole,2-(1,1-dimethylethyl)-

Inchi: InChI=1S/C8H13N/c1-8(2,3)7-5-4-6-9-7/h4-6,9H,1-3H3
InchiKey: AJPCQTXGHLEGAY-UHFFFAOYSA-N
Formula: C8H13N
SMILES: CC(C)(C)c1ccc[nH]1
Mol. weight [g/mol]: 123.20
CAS: 5398-58-3

Physical Properties

Property code	Value	Unit	Source
ie	7.95 ± 0.05	eV	NIST Webbook
log10ws	-2.00		Crippen Method
logp	1.830		Crippen Method
mcvol	114.100	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=C5398583&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.