1H-Pyrrole, 2-pentyl

Other names: Pyrrole, 2-pentyl
Inchi: InChI=1S/C9H15N/c1-2-3-4-6-9-7-5-8-10-9/h5,7-8,10H,2-4,6H2,1H3
InchiKey: SBEGSTRVXAZUOJ-UHFFFAOYSA-N
Formula: C9H15N
SMILES: CCCCCc1ccc[nH]1
Mol. weight [g/mol]: 137.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.75		Crippen Method
logp	2.265		Crippen Method
mcvol	128.190	ml/mol	McGowan Method
rinpol	1040.00		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=R62417&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

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