

1H-Pyrrole, 1-methyl-2-pentyl

Inchi: InChI=1S/C10H17N/c1-3-4-5-7-10-8-6-9-11(10)2/h6,8-9H,3-5,7H2,1-2H3
InchiKey: GVZIOFGTDMVMSK-UHFFFAOYSA-N
Formula: C10H17N
SMILES: CCCCCc1cccn1C
Mol. weight [g/mol]: 151.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.82		Crippen Method
logp	2.758		Crippen Method
mcvol	142.280	ml/mol	McGowan Method
rinpol	1252.00		NIST Webbook
rinpol	1252.00		NIST Webbook
rinpol	1252.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R62962&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

Latest version available from:

<https://www.chemeo.com/cid/55-598-8/1H-Pyrrole-1-methyl-2-pentyl.pdf>

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