

1H-Pyrrole, 1-pentyl-

Other names:	Pyrrole, 1-pentyl- N-Amylpyrrole 1-Amylpyrrole
Inchi:	InChI=1S/C9H15N/c1-2-3-4-7-10-8-5-6-9-10/h5-6,8-9H,2-4,7H2,1H3
InchiKey:	VODBTJROPIJKCF-UHFFFAOYSA-N
Formula:	C9H15N
SMILES:	CCCCCn1cccc1
Mol. weight [g/mol]:	137.22
CAS:	699-22-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.99		Crippen Method
logp	2.678		Crippen Method
mcvol	128.190	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C699229&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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<https://www.chemeo.com/cid/54-448-5/1H-Pyrrole-1-pentyl.pdf>

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