

1H-Pyrrole, 3-ethyl-

Other names:	3-ethyl-1H-pyrrole
Inchi:	InChI=1S/C6H9N/c1-2-6-3-4-7-5-6/h3-5,7H,2H2,1H3
InchiKey:	RLLBWIDEGAIFPI-UHFFFAOYSA-N
Formula:	C6H9N
SMILES:	CCc1cc[nH]c1
Mol. weight [g/mol]:	95.14
CAS:	1551-16-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.49		Crippen Method
logp	1.095		Crippen Method
mcvol	85.920	ml/mol	McGowan Method
ripol	950.00		NIST Webbook
ripol	950.00		NIST Webbook
ripol	1657.00		NIST Webbook
ripol	1617.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1551162&Units=SI
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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ripol:	Non-polar retention indices

ripol: Polar retention indices

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<https://www.chemeo.com/cid/44-037-2/1H-Pyrrole-3-ethyl.pdf>

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