

1H-Pyrrole, 3-ethyl-2,5-dimethyl-

Other names:	3-ethyl-2,5-dimethyl-1H-pyrrole
Inchi:	InChI=1S/C8H13N/c1-4-8-5-6(2)9-7(8)3/h5,9H,4H2,1-3H3
InchiKey:	MSXUEMBOMBOMG-UHFFFAOYSA-N
Formula:	C8H13N
SMILES:	CCc1cc(C)[nH]c1C
Mol. weight [g/mol]:	123.20
CAS:	69687-78-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.44		Crippen Method
logp	1.712		Crippen Method
mcvol	114.100	ml/mol	McGowan Method
rinpol	1119.00		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=C69687781&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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<https://www.chemeo.com/cid/44-219-0/1H-Pyrrole-3-ethyl-2-5-dimethyl.pdf>

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