

1H-Pyrrole, 2,3-dimethyl-

Other names:	2,3-dimethyl-1H-pyrrole
Inchi:	InChI=1S/C6H9N/c1-5-3-4-7-6(5)2/h3-4,7H,1-2H3
InchiKey:	OUYLXVQKVVBXUGW-UHFFFAOYSA-N
Formula:	C6H9N
SMILES:	Cc1cc[nH]c1C
Mol. weight [g/mol]:	95.14
CAS:	600-28-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.64		Crippen Method
logp	1.150		Crippen Method
mcvol	85.920	ml/mol	McGowan Method
rinpola	804.00		NIST Webbook
ripola	1620.00		NIST Webbook
ripol	1620.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C600282&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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/67-113-2/1H-Pyrrole-2-3-dimethyl.pdf>

Generated by Cheméo on 2024-04-28 19:24:02.595006835 +0000 UTC m=+16621491.515584151.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.