

1H-Pyrrole, 2,5-dimethyl-1-phenyl-

Other names:	Pyrrole, 2,5-dimethyl-1-phenyl- 2,5-Dimethyl-1-phenylpyrrole 1-Phenyl-2,5-dimethylpyrrole 2,5-dimethyl-1-phenyl-1H-pyrrole
Inchi:	InChI=1S/C12H13N/c1-10-8-9-11(2)13(10)12-6-4-3-5-7-12/h3-9H,1-2H3
InchiKey:	JNXIFVSGXLGULI-UHFFFAOYSA-N
Formula:	C12H13N
SMILES:	<chem>Cc1ccc(C)n1-c1ccccc1</chem>
Mol. weight [g/mol]:	171.24
CAS:	83-24-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.07		Crippen Method
logp	3.094		Crippen Method
mcvol	146.700	ml/mol	McGowan Method
tf	322.65 ± 1.50	K	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=C83249&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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