

1H-Pyrrole, 1-phenyl-

Other names:	1-phenylpyrrole N-phenylpyrrole Pyrrole, 1-phenyl- pyrrole, N-phenyl-
Inchi:	InChI=1S/C10H9N/c1-2-6-10(7-3-1)11-8-4-5-9-11/h1-9H
InchiKey:	GEZGAZKEOUKLBR-UHFFFAOYSA-N
Formula:	C10H9N
SMILES:	c1ccc(-n2cccc2)cc1
Mol. weight [g/mol]:	143.19
CAS:	635-90-5

Physical Properties

Property code	Value	Unit	Source
hfus	80.80	kJ/mol	Experimental and computational thermochemistry of 1-phenylpyrrole and 1-(4-methylphenyl)pyrrole
log10ws	-3.12		Crippen Method
logp	2.477		Crippen Method
mcvol	118.520	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Experimental and computational thermochemistry of 1-phenylpyrrole and 1-(4-methylphenyl)pyrrole:	https://www.doi.org/10.1016/j.jct.2010.01.009
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C635905&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hfus: Enthalpy of fusion at standard conditions

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

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