

# 1-(4-Iodophenyl)pyrrole

<b>Inchi:</b>	InChI=1S/C10H8IN/c11-9-3-5-10(6-4-9)12-7-1-2-8-12/h1-8H
<b>InchiKey:</b>	FMURNAZHVQDQQN-UHFFFAOYSA-N
<b>Formula:</b>	C10H8IN
<b>SMILES:</b>	<chem>Ic1ccc(-n2cccc2)cc1</chem>
<b>Mol. weight [g/mol]:</b>	269.08
<b>CAS:</b>	92636-36-7

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.27		Crippen Method
logp	3.082		Crippen Method
mcpvol	144.340	ml/mol	McGowan Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
psub	1.07e-04	kPa	319.11	A calorimetric and computational study of the thermochemistry of halogenated 1-phenylpyrrole derivatives
psub	1.12e-04	kPa	319.11	A calorimetric and computational study of the thermochemistry of halogenated 1-phenylpyrrole derivatives
psub	1.09e-04	kPa	319.11	A calorimetric and computational study of the thermochemistry of halogenated 1-phenylpyrrole derivatives

psub	1.42e-04	kPa	321.19	A calorimetric and computational study of the thermochemistry of halogenated 1-phenylpyrrole derivatives
psub	1.40e-04	kPa	321.19	A calorimetric and computational study of the thermochemistry of halogenated 1-phenylpyrrole derivatives
psub	1.37e-04	kPa	321.19	A calorimetric and computational study of the thermochemistry of halogenated 1-phenylpyrrole derivatives
psub	1.74e-04	kPa	323.18	A calorimetric and computational study of the thermochemistry of halogenated 1-phenylpyrrole derivatives
psub	1.69e-04	kPa	323.18	A calorimetric and computational study of the thermochemistry of halogenated 1-phenylpyrrole derivatives
psub	1.69e-04	kPa	323.18	A calorimetric and computational study of the thermochemistry of halogenated 1-phenylpyrrole derivatives
psub	2.10e-04	kPa	325.12	A calorimetric and computational study of the thermochemistry of halogenated 1-phenylpyrrole derivatives

psub	2.18e-04	kPa	325.12	A calorimetric and computational study of the thermochemistry of halogenated 1-phenylpyrrole derivatives
psub	2.16e-04	kPa	325.12	A calorimetric and computational study of the thermochemistry of halogenated 1-phenylpyrrole derivatives
psub	2.74e-04	kPa	327.19	A calorimetric and computational study of the thermochemistry of halogenated 1-phenylpyrrole derivatives
psub	2.70e-04	kPa	327.19	A calorimetric and computational study of the thermochemistry of halogenated 1-phenylpyrrole derivatives
psub	2.65e-04	kPa	327.19	A calorimetric and computational study of the thermochemistry of halogenated 1-phenylpyrrole derivatives
psub	3.36e-04	kPa	329.18	A calorimetric and computational study of the thermochemistry of halogenated 1-phenylpyrrole derivatives
psub	3.31e-04	kPa	329.18	A calorimetric and computational study of the thermochemistry of halogenated 1-phenylpyrrole derivatives

psub	3.29e-04	kPa	329.18	A calorimetric and computational study of the thermochemistry of halogenated 1-phenylpyrrole derivatives
psub	4.02e-04	kPa	331.11	A calorimetric and computational study of the thermochemistry of halogenated 1-phenylpyrrole derivatives
psub	4.21e-04	kPa	331.11	A calorimetric and computational study of the thermochemistry of halogenated 1-phenylpyrrole derivatives
psub	4.16e-04	kPa	331.11	A calorimetric and computational study of the thermochemistry of halogenated 1-phenylpyrrole derivatives
psub	5.20e-04	kPa	333.17	A calorimetric and computational study of the thermochemistry of halogenated 1-phenylpyrrole derivatives
psub	5.22e-04	kPa	333.17	A calorimetric and computational study of the thermochemistry of halogenated 1-phenylpyrrole derivatives
psub	5.08e-04	kPa	333.17	A calorimetric and computational study of the thermochemistry of halogenated 1-phenylpyrrole derivatives

psub	6.39e-04	kPa	335.17	A calorimetric and computational study of the thermochemistry of halogenated 1-phenylpyrrole derivatives
psub	6.28e-04	kPa	335.17	A calorimetric and computational study of the thermochemistry of halogenated 1-phenylpyrrole derivatives
psub	6.24e-04	kPa	335.17	A calorimetric and computational study of the thermochemistry of halogenated 1-phenylpyrrole derivatives
psub	7.78e-04	kPa	337.12	A calorimetric and computational study of the thermochemistry of halogenated 1-phenylpyrrole derivatives
psub	8.14e-04	kPa	337.12	A calorimetric and computational study of the thermochemistry of halogenated 1-phenylpyrrole derivatives
psub	8.06e-04	kPa	337.12	A calorimetric and computational study of the thermochemistry of halogenated 1-phenylpyrrole derivatives
psub	1.02e-03	kPa	339.19	A calorimetric and computational study of the thermochemistry of halogenated 1-phenylpyrrole derivatives

psub	1.01e-03	kPa	339.19	A calorimetric and computational study of the thermochemistry of halogenated 1-phenylpyrrole derivatives
psub	9.77e-04	kPa	339.19	A calorimetric and computational study of the thermochemistry of halogenated 1-phenylpyrrole derivatives
psub	1.24e-03	kPa	341.17	A calorimetric and computational study of the thermochemistry of halogenated 1-phenylpyrrole derivatives
psub	1.21e-03	kPa	341.17	A calorimetric and computational study of the thermochemistry of halogenated 1-phenylpyrrole derivatives
psub	1.21e-03	kPa	341.17	A calorimetric and computational study of the thermochemistry of halogenated 1-phenylpyrrole derivatives

## Sources

Crippen Method:

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

A calorimetric and computational study of the thermochemistry of halogenated 1-phenylpyrrole derivatives :

<https://www.doi.org/10.1016/j.jct.2010.06.012>

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C92636367&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

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

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