

1-(4-Iodophenyl)pyrrole

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C92636367&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: 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>

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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