

1-(2-Nitrophenyl)pyrrole

Inchi:	InChI=1S/C10H8N2O2/c13-12(14)10-6-2-1-5-9(10)11-7-3-4-8-11/h1-8H
InchiKey:	UQNRTIQRQZGKL-UHFFFAOYSA-N
Formula:	C10H8N2O2
SMILES:	O=[N+](O)c1cccc1-n1cccc1
Mol. weight [g/mol]:	188.18
CAS:	33265-60-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.77		Crippen Method
logp	2.385		Crippen Method
mcvol	135.940	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	101.30	kJ/mol	298.15	A joint experimental and computational investigation on the thermochemistry of (nitrophenyl)pyrroles

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33265600&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
A joint experimental and computational investigation on the thermochemistry of (nitrophenyl)pyrroles:	https://www.doi.org/10.1016/j.jct.2010.03.021

Legend

hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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