1-(p-NITROPHENYL)PYRROLE

Other names: 1-(4-nitrophenyl)pyrrole
Inchi: InChI=1S/C10H8N2O2/c13-12(14)10-5-3-9(4-6-10)11-7-1-2-8-11/h1-8H
InchiKey: PWCFKNYSCGRNRW-UHFFFAOYSA-N
Formula: C10H8N2O2
SMILES: O=[N+]([O-])c1ccc(-n2cccc2)cc1
Mol. weight [g/mol]: 188.19

Physical Properties

Property code	Value	Unit	Source
hf	193.61	kJ/mol	Cheméo Relay (1.0)
hvap	91.89	kJ/mol	Cheméo Relay (1.0)
ie	8.44	eV	Cheméo Relay (1.0)
log10ws	-3.54		Cheméo Relay (1.0)
logp	2.385		Crippen Method
mcvol	135.940	ml/mol	McGowan Method
tb	592.29	K	Cheméo Relay (1.0)
tf	408.72	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	109.60	kJ/mol	355.13	A joint experimental and computational investigation on the thermochemistry of (nitrophenyl)pyrroles

Sources

Cheméo Relay (1.0, beta):

A joint experimental and computational investigation on the thermochemistry of (nitrophenyl)pyrroles:	https://www.doi.org/10.1016/j.jct.2010.03.021
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4533420&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point