

1-(P-NITROPHENYL)PIPERIDINE

Other names:	1-(4-nitrophenyl)piperidine
Inchi:	InChI=1S/C11H14N2O2/c14-13(15)11-6-4-10(5-7-11)12-8-2-1-3-9-12/h4-7H,1-3,8-9H2
InchiKey:	SGPLAXFUDTWHRS-UHFFFAOYSA-N
Formula:	C11H14N2O2
SMILES:	O=[N+]([O-])c1ccc(N2CCCCC2)cc1
Mol. weight [g/mol]:	206.25

Physical Properties

Property code	Value	Unit	Source
hf	25.23	kJ/mol	Cheméo Relay (1.0)
hvap	84.30	kJ/mol	Cheméo Relay (1.0)
ie	7.96	eV	Cheméo Relay (1.0)
log10ws	-3.63		Cheméo Relay (1.0)
logp	2.585		Crippen Method
mcvol	158.630	ml/mol	McGowan Method
tb	597.96	K	Cheméo Relay (1.0)
tf	375.65 ± 2.00	K	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C6574158&Units=SI>

McGowan Method:

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

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf: Enthalpy of formation at standard conditions

hvap: Enthalpy of vaporization at standard conditions

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

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