

N''-(4-iodo-phenyl)-N,N,N',N'-tetramethyl-guanidine

Inchi:	InChI=1S/C11H16IN3/c1-14(2)11(15(3)4)13-10-7-5-9(12)6-8-10/h5-8H,1-4H3
InchiKey:	FWJQSWBHYJMHLG-UHFFFAOYSA-N
Formula:	C11H16IN3
SMILES:	CN(C)C(=Nc1ccc(I)cc1)N(C)C
Mol. weight [g/mol]:	317.17

Physical Properties

Property code	Value	Unit	Source
hf	239.05	kJ/mol	Joback Method
hvap	59.87	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	2.402		Crippen Method
mcvol	193.550	ml/mol	McGowan Method
pc	2302.53	kPa	Joback Method
tb	677.32	K	Joback Method
tc	922.16	K	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R153061&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature

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