N''-(3-fluoro-phenyl)-N,N,N',N'-tetramethyl-guanidine

Inchi: InChI=1S/C11H16FN3/c1-14(2)11(15(3)4)13-10-7-5-6-9(12)8-10/h5-8H,1-4H3
InchiKey: XZICHZWUZQTBRA-UHFFFAOYSA-N
Formula: C11H16FN3
SMILES: CN(C)C(=Nc1cccc(F)c1)N(C)C
Mol. weight [g/mol]: 209.26

Physical Properties

Property code	Value	Unit	Source
hf	-33.93	kJ/mol	Joback Method
hvap	49.68	kJ/mol	Joback Method
log10ws	-1.76		Crippen Method
logp	1.936		Crippen Method
mcvol	169.500	ml/mol	McGowan Method
pc	2252.53	kPa	Joback Method
rinpol	1556.00		NIST Webbook
tb	583.45	K	Joback Method
tc	791.72	K	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R152984&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature