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

Inchi: InChI=1S/C13H21N3O/c1-6-17-12-9-7-8-11(10-12)14-13(15(2)3)16(4)5/h7-10H,6H2,1-5H

InchiKey: KEINSPTYZUKPIE-UHFFFAOYSA-N

Formula: C13H21N3O

SMILES: CCOc1cccc(N=C(N(C)C)N(C)C)c1

Mol. weight [g/mol]: 235.33

Physical Properties

Property code	Value	Unit	Source
hf	-11.32	kJ/mol	Joback Method
hvap	57.36	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	2.196		Crippen Method
mcvol	201.780	ml/mol	McGowan Method
pc	1938.95	kPa	Joback Method
rinpol	1801.00		NIST Webbook
rinpol	1801.00		NIST Webbook
tb	652.36	K	Joback Method
tc	861.41	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=R152979&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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