Benzamidine, 4-(3-butyl-3-methyl-1-triazenol)-

Inchi: InChI=1S/C12H19N5/c1-3-4-9-17(2)16-15-11-7-5-10(6-8-11)12(13)14/h5-8H,3-4,9H2,1-2
InchiKey: KGBJMOVDNODQFS-FOCLMDBBSA-N
Formula: C12H19N5
SMILES: CCCCN(C)N=Nc1ccc(C(=N)N)cc1
Mol. weight [g/mol]: 233.31
CAS: 116557-74-5

Physical Properties

Property code	Value	Unit	Source
hf	280.92	kJ/mol	Joback Method
hvap	76.68	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	2.701		Crippen Method
mcvol	197.480	ml/mol	McGowan Method
tb	824.13	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116557745&Units=SI
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

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

tb: Normal Boiling Point Temperature