

Imidazole-4-carboxamide, 5-(3,3-dibenzyltriazeno)-

Inchi:	InChI=1S/C18H18N6O/c19-17(25)16-18(21-13-20-16)22-23-24(11-14-7-3-1-4-8-14)12-15
InchiKey:	WWFLLHQESZUYRL-GHVJWSGMSA-N
Formula:	C18H18N6O
SMILES:	NC(=O)c1nc[nH]c1N=NN(Cc1ccccc1)Cc1ccccc1
Mol. weight [g/mol]:	334.38
CAS:	6939-30-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.07		Crippen Method
logp	2.728		Crippen Method
mcvol	254.650	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6939306&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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