

5-(3',3'-Dibutyl-1'-triazeno)-1,2,3-triazole-4-carboxamide

Inchi:	InChI=1S/C11H21N7O/c1-3-5-7-18(8-6-4-2)17-15-11-9(10(12)19)13-16-14-11/h3-8H2,1-
InchiKey:	WERLXODHIIOZOS-BMRADRMJSA-N
Formula:	C11H21N7O
SMILES:	CCCCN(CCCC)N=Nc1[nH]nnc1C(N)=O
Mol. weight [g/mol]:	267.33
CAS:	4342-10-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.13		Crippen Method
logp	1.323		Crippen Method
mcvol	213.520	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4342103&Units=SI
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

Legend

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

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