

4-Imidazolecarboxamide, 5-(butyl-1-triazeno)-

Inchi:	InChI=1S/C8H14N6O/c1-2-3-4-12-14-13-8-6(7(9)15)10-5-11-8/h5H,2-4H2,1H3,(H2,9,15)
InchiKey:	OPJQRGVUQOTCSJ-UHFFFAOYSA-N
Formula:	C8H14N6O
SMILES:	CCCCNN=Nc1[nH]cnc1C(N)=O
Mol. weight [g/mol]:	210.24
CAS:	3413-74-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.31		Crippen Method
logp	0.415		Crippen Method
mcvol	161.270	ml/mol	McGowan Method

Sources

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=C3413749&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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