

# 1H-1,2,3-triazole-4-carboxamide, 5-[3-(p-bromophenyl)-1-triazeno]-

Inchi:	InChI=1S/C9H8BrN7O/c10-5-1-3-6(4-2-5)12-16-14-9-7(8(11)18)13-17-15-9/h1-4H,(H2,1)
InchiKey:	MJIHKQOPKHLWJE-UHFFFAOYSA-N
Formula:	C9H8BrN7O
SMILES:	NC(=O)c1nn[nH]c1N=NNc1ccc(Br)cc1
Mol. weight [g/mol]:	310.11
CAS:	7229-15-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.61		Crippen Method
logp	1.295		Crippen Method
mcvol	179.080	ml/mol	McGowan Method

## Sources

Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C7229154&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C7229154&amp;Units=SI</a>

## Legend

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

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