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,(H2,11

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: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=C7229154&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume