

1H-1,2,3-triazole-4-carboxamide, 5-(1-pyrrolidinylazo)-

Inchi:	InChI=1S/C7H11N7O/c8-6(15)5-7(10-12-9-5)11-13-14-3-1-2-4-14/h1-4H2,(H2,8,15)(H,9,
InchiKey:	QBTZNGLFEEKKOC-ACCUITESSA-N
Formula:	C7H11N7O
SMILES:	NC(=O)c1nn[nH]c1N=NN1CCCC1
Mol. weight [g/mol]:	209.21
CAS:	7229-10-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.35		Crippen Method
logp	-0.484		Crippen Method
mcvol	146.300	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7229109&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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