

Triazole-4-carboxamide, (1h)-1,2,3-, 5-[(n-methyl-n-phenyl)-1-triazeno]-

Inchi:	InChI=1S/C10H11N7O/c1-17(7-5-3-2-4-6-7)16-14-10-8(9(11)18)12-15-13-10/h2-6H,1H3,
InchiKey:	KDOOWDLMNDCJMW-JQIJEIRASA-N
Formula:	C10H11N7O
SMILES:	CN(N=Nc1[nH]nnc1C(N)=O)c1ccccc1
Mol. weight [g/mol]:	245.24
CAS:	7229-14-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.35		Crippen Method
logp	0.557		Crippen Method
mcvol	175.670	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=C7229143&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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