

Purine, 2-azido-

Inchi:	InChI=1S/C5H3N7/c6-12-11-5-7-1-3-4(10-5)9-2-8-3/h1-2H,(H,7,8,9,10)
InchiKey:	ICHLNDWMYWZUTG-UHFFFAOYSA-N
Formula:	C5H3N7
SMILES:	[N-]=[N+]=Nc1ncc2[nH]cnc2n1
Mol. weight [g/mol]:	161.12
CAS:	7086-36-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.45		Crippen Method
logp	0.813		Crippen Method
mcvol	103.650	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=C7086364&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/77-727-0/Purine-2-azido.pdf>

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