1H-1,2,3-Triazole

Other names:	V-triazole
	Osotriazole
	Pyrrodiazole
	Triazacyclopentadiene
	1,2,3-Triazole
Inchi:	InChI=1S/C2H3N3/c1-2-4-5-3-1/h1-2H,(H,3,4,5)
InchiKey:	QWENRTYMTSOGBR-UHFFFAOYSA-N
Formula:	C2H3N3
SMILES:	c1c[nH]nn1
Mol. weight [g/mol]:	69.07
CAS:	288-36-8

Physical Properties

Property code	Value	Unit	Source
affp	879.30	kJ/mol	NIST Webbook
basg	847.40	kJ/mol	NIST Webbook
ie	10.06	eV	NIST Webbook
ie	10.10	eV	NIST Webbook
log10ws	-0.22		Crippen Method
logp	-0.677		Crippen Method
mcvol	49.520	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=C288368&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume