1H-1,2,3-Triazole, 4-phenyl-

Other names:	v-Triazole, 4-phenyl-
	4-Phenyl-1H-1,2,3-triazole
	4-Phenyl-1,2,3-triazole
Inchi:	InChI=1S/C8H7N3/c1-2-4-7(5-3-1)8-6-9-11-10-8/h1-6H,(H,9,10,11)
InchiKey:	LUEYUHCBBXWTQT-UHFFFAOYSA-N
Formula:	C8H7N3
SMILES:	c1ccc(-c2c[nH]nn2)cc1
Mol. weight [g/mol]:	145.16
CAS:	1680-44-0

Physical Properties

Property code	Value	Unit	Source
chs	-4296.50	kJ/mol	NIST Webbook
log10ws	-2.83		Crippen Method
logp	0.990		Crippen Method
mcvol	110.300	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=C1680440&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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