p-(1H-1,2,4-Triazol-1-yl) phenol

Other names:	4-(1,2,4-Triazol-1-yl)phenol
	Phenol, 4-(1H-1,2,4-triazol-1-yl)-
	4-(1H-1,2,4-triazol-1-yl)phenol
Inchi:	InChI=1S/C8H7N3O/c12-8-3-1-7(2-4-8)11-6-9-5-10-11/h1-6,12H
InchiKey:	ZOPIBCDDKMAEII-UHFFFAOYSA-N
Formula:	C8H7N3O
SMILES:	Oc1ccc(-n2cncn2)cc1
Mol. weight [g/mol]:	161.16
CAS:	68337-15-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.20		Crippen Method
logp	0.973		Crippen Method
mcvol	116.170	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=C68337155&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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