Phenol, 2-[(1H-1,2,4-triazol-3-ylimino)methyl]-

Other names:	Phenol, o-(N-S-triazol-3-ylformimidoyl)-
	Phenol, 2-(1,2,4-triazol-3-yliminomethyl)-
	1,2,4-Triazole, 3-(sigma-hydroxybenzylidene)amino-
Inchi:	InChI=1S/C9H8N4O/c14-8-4-2-1-3-7(8)5-10-9-11-6-12-13-9/h1-6,14H,(H,11,12,13)
InchiKey:	BKYHBHVZLQLDIP-UHFFFAOYSA-N
Formula:	C9H8N4O
SMILES:	Oc1ccccc1C=Nc1ncn[nH]1
Mol. weight [g/mol]:	188.19
CAS:	24829-12-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.64		Crippen Method
logp	0.779		Crippen Method
mcvol	135.940	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24829127&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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