1-Phenyl-5-hydroxytetrazole

Inchi: InChI=1S/C7H6N4O/c12-7-8-9-10-11(7)6-4-2-1-3-5-6/h1-5H,(H,8,10,12)
InchiKey: FYYACQQSYSDVJB-UHFFFAOYSA-N
Formula: C7H6N4O
SMILES: Oc1nnnn1-c1ccccc1
Mol. weight [g/mol]: 162.15
CAS: 51449-77-5

Physical Properties

Property code	Value	Unit	Source
chs	-3723.80 ± 2.80	kJ/mol	NIST Webbook
hfs	111.80	kJ/mol	NIST Webbook
log10ws	-1.97		Crippen Method
logp	0.368		Crippen Method
mcvol	112.060	ml/mol	McGowan Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C51449775&Units=SI

Legend

chs: Standard solid enthalpy of combustion
hfs: Solid phase enthalpy of formation at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume