2-Phenyl-5-methyltetrazole

Inchi: InChI=1S/C8H8N4/c1-7-9-11-12(10-7)8-5-3-2-4-6-8/h2-6H,1H3
InchiKey: DWFDADZCRATSDV-UHFFFAOYSA-N
Formula: C8H8N4
SMILES: Cc1nnn(-c2ccccc2)n1
Mol. weight [g/mol]: 160.18
CAS: 22706-20-3

Physical Properties

Property code	Value	Unit	Source
chs	-4566.04 ± 0.59	kJ/mol	NIST Webbook
hfs	274.60	kJ/mol	NIST Webbook
log10ws	-2.90		Crippen Method
logp	0.971		Crippen Method
mcvol	120.280	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C22706203&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

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

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