5-PHENYL-1H-TETRAZOLE

Inchi: InChI=1S/C7H6N4/c1-2-4-6(5-3-1)7-8-10-11-9-7/h1-5H,(H,8,9,10,11)
InchiKey: MARUHZGHZWCEQU-UHFFFAOYSA-N
Formula: C7H6N4
SMILES: c1ccc(-c2nnn[nH]2)cc1
Mol. weight [g/mol]: 146.15

Physical Properties

Property code	Value	Unit	Source
hf	453.16	kJ/mol	Cheméo Relay (1.0)
logp	0.385		Crippen Method
mcvol	106.190	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
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C18039424&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

hf: Enthalpy of formation at standard conditions
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume