cis-2,2'-Dimethyl-5,5'-azotetrazole

Inchi: InChI=1S/C4H6N10/c1-13-3(7-9-11-13)5-6-4-8-10-12-14(4)2/h1-2H3/b6-5-
InchiKey: HOXMAHGFAGMFCJ-WAYWQWQTSA-N
Formula: C4H6N10
SMILES: Cn1nnnc1N=Nc1nnnn1C
Mol. weight [g/mol]: 194.16
CAS: 41463-69-8

Physical Properties

Property code	Value	Unit	Source
chs	-3186.20 ± 4.60	kJ/mol	NIST Webbook
hfs	754.60 ± 4.60	kJ/mol	NIST Webbook
log10ws	-4.68		Crippen Method
logp	-0.851		Crippen Method
mcvol	123.800	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C41463698&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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