

# 5,5'-Bitetrazole

**Inchi:** InChI=1S/C2H2N8/c3-1(4-8-7-3)2-5-9-10-6-2/h(H,3,4,7,8)(H,5,6,9,10)  
**InchiKey:** MTAYYBKXNAEQOK-UHFFFAOYSA-N  
**Formula:** C2H2N8  
**SMILES:** n1n[nH]c(-c2nnn[nH]2)n1  
**Mol. weight [g/mol]:** 138.09  
**CAS:** 2783-98-4

## Physical Properties

Property code	Value	Unit	Source
chs	-1604.60 ± 0.96	kJ/mol	NIST Webbook
hfs	531.70 ± 0.96	kJ/mol	NIST Webbook
hfs	531.70	kJ/mol	NIST Webbook
log10ws	-1.11		Crippen Method
logp	-2.584		Crippen Method
mcvol	79.960	ml/mol	McGowan Method

## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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=C2783984&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## 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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