

5-Phenylaminotetrazole

Inchi: InChI=1S/C7H7N5/c1-2-4-6(5-3-1)8-7-9-11-12-10-7/h1-5H,(H2,8,9,10,11,12)
InchiKey: JJGVUQXLNNGWPZ-UHFFFAOYSA-N
Formula: C7H7N5
SMILES: c1ccc(Nc2nnn[nH]2)cc1
Mol. weight [g/mol]: 161.16
CAS: 23579-46-6

Physical Properties

Property code	Value	Unit	Source
chs	-4060.00 ± 0.08	kJ/mol	NIST Webbook
hfs	305.00	kJ/mol	NIST Webbook
log10ws	-1.79		Crippen Method
logp	0.461		Crippen Method
mcvol	116.170	ml/mol	McGowan Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=C23579466&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

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