

Benzal 3-hydrazino-5-methyl-1,2,4-triazol

Inchi: InChI=1S/C10H11N5/c1-8-12-10(15-13-8)14-11-7-9-5-3-2-4-6-9/h2-7H,1H3,(H2,12,13,14)
InchiKey: MYKANLIJGNQWPO-YRNVUSSQSA-N
Formula: C10H11N5
SMILES: Cc1nc(NN=Cc2ccccc2)n[nH]1
Mol. weight [g/mol]: 201.23
CAS: 87123-46-4

Physical Properties

Property code	Value	Unit	Source
chs	-5765.00 ± 1.00	kJ/mol	NIST Webbook
hfs	257.70	kJ/mol	NIST Webbook
log10ws	-2.58		Crippen Method
logp	1.077		Crippen Method
mcvol	154.140	ml/mol	McGowan Method

Sources

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=C87123464&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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