3-Tetrazene-2-carboximidamide, 4-(1H-tetrazol-5-yl)-,monohydrate

Other names: 3-Tetrazene-2-carboximidamide, 4-(2H-tetrazol-5-yl)-, hydrate (1:1)
tetrazene
Inchi: InChI=1S/C2H6N10/c3-1(4)12(5)11-8-2-6-9-10-7-2/h5H2,(H3,3,4)(H,6,7,9,10)/b11-8+
InchiKey: WSLWDHGXSGRREP-DHZHZOJOSA-N
Formula: C2H6N10.H2O
SMILES: N=C(N)N(N)N=Nc1nnn[nH]1
Mol. weight [g/mol]: 188.15
CAS: 31330-63-9

Physical Properties

Property code	Value	Unit	Source
chs	-2120.00 ± 3.00	kJ/mol	NIST Webbook
hfs	189.00 ± 3.00	kJ/mol	NIST Webbook
log10ws	-1.56		Crippen Method
logp	-2.214		Crippen Method
mcvol	110.780	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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C31330639&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