3H-1,2,4-Triazol-3-one, 1,2-dihydro-

Other names: s-Triazol-3-ol
1,2-dihydro-3H-1,2,4-triazol-3-one
Inchi: InChI=1S/C2H3N3O/c6-2-3-1-4-5-2/h1H,(H2,3,4,5,6)
InchiKey: LZTSCEYDCZBRCJ-UHFFFAOYSA-N
Formula: C2H3N3O
SMILES: O=c1[nH]cn[nH]1
Mol. weight [g/mol]: 85.06
CAS: 930-33-6

Physical Properties

Property code	Value	Unit	Source
chs	-1073.34 ± 0.59	kJ/mol	NIST Webbook
hfs	-142.40 ± 0.70	kJ/mol	NIST Webbook
ie	9.18	eV	NIST Webbook
log10ws	0.90		Crippen Method
logp	-1.866		Crippen Method
mcvol	55.390	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	68.90	J/mol×K	320.00	NIST Webbook

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=C930336&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cps:	Solid phase heat capacity
hfs:	Solid phase enthalpy of formation at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume