1H-Tetrazole, 1-phenyl-

Other names: 1-Phenyl-1H-tetrazole
1-Phenyltetrazole
Inchi: InChI=1S/C7H6N4/c1-2-4-7(5-3-1)11-6-8-9-10-11/h1-6H
InchiKey: IYPXPGSELZFFMI-UHFFFAOYSA-N
Formula: C7H6N4
SMILES: c1ccc(-n2cnnn2)cc1
Mol. weight [g/mol]: 146.15
CAS: 5378-52-9

Physical Properties

Property code	Value	Unit	Source
chs	-3973.90 ± 1.50	kJ/mol	NIST Webbook
chs	-3956.00 ± 0.40	kJ/mol	NIST Webbook
hf	448.00 ± 3.00	kJ/mol	NIST Webbook
hf	465.80	kJ/mol	NIST Webbook
hfs	344.00 ± 0.40	kJ/mol	NIST Webbook
hfs	361.80	kJ/mol	NIST Webbook
hsub	104.00 ± 3.00	kJ/mol	NIST Webbook
hsub	104.00	kJ/mol	NIST Webbook
log10ws	-2.42		Crippen Method
logp	0.662		Crippen Method
mcvol	106.190	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5378529&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume