1H-Tetrazole, 5-phenyl-

Other names:	2H-Tetrazole, 5-phenyl- 5-Phenyl tetrazole 5-Phenyl(1H)tetrazole 5-Phenyl-2H-tetrazole 5-phenyltetrazole MA 1623
Inchi:	InChI=1S/C7H6N4/c1-2-4-6(5-3-1)7-8-10-11-9-7/h1-5H,(H,8,9,10,11)
InchiKey:	MARUHZGHZWCEQU-UHFFFAOYSA-N
Formula:	C7H6N4
SMILES:	c1ccc(-c2nnn[nH]2)cc1
Mol. weight [g/mol]:	146.15
CAS:	18039-42-4

Physical Properties

Property code	Value	Unit	Source
chs	-3904.60 ± 1.40	kJ/mol	NIST Webbook
chs	-3910.00 ± 3.00	kJ/mol	NIST Webbook
hf	413.00 ± 5.90	kJ/mol	NIST Webbook
hf	407.50	kJ/mol	NIST Webbook
hfs	298.00 ± 3.00	kJ/mol	NIST Webbook
hfs	292.50	kJ/mol	NIST Webbook
hsub	115.00 ± 3.00	kJ/mol	NIST Webbook
hsub	115.00	kJ/mol	NIST Webbook
log10ws	-2.59		Crippen Method
logp	0.385		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=C18039424&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility modelling and dissolution properties of 5-phenyltetrazole in thirteen mono-solvents and liquid mixtures of (methanol + ethyl acetate) at elevated temperatures:	https://www.doi.org/10.1016/j.jct.2017.04.019

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