1-Methyl-5-phenyltetrazole

Other names:	Tetrazole, 1-methyl-5-phenyl- 1H-Tetrazole, 1-methyl-5-phenyl-
Inchi:	InChI=1S/C8H8N4/c1-12-8(9-10-11-12)7-5-3-2-4-6-7/h2-6H,1H3
InchiKey:	UIEGWLAONRMBOG-UHFFFAOYSA-N
Formula:	C8H8N4
SMILES:	Cn1nnnc1-c1ccccc1
Mol. weight [g/mol]:	160.18
CAS:	20743-50-4

Physical Properties

Property code	Value	Unit	Source
chs	-4583.70 ± 1.30	kJ/mol	NIST Webbook
hfs	292.20 ± 1.30	kJ/mol	NIST Webbook
log10ws	-4.66		Crippen Method
logp	0.877		Crippen Method
mcvol	120.280	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=C20743504&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
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