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

Physical Properties

Property code	Value	Unit	Source
chs	-4583.70 ± 1.30	kJ/mol	NIST Webbook
hf	436.93	kJ/mol	Cheméo Relay (1.0)
hfs	292.20 ± 1.30	kJ/mol	NIST Webbook
hvap	91.79	kJ/mol	Cheméo Relay (1.0)
logp	0.877		Crippen Method
mcvol	120.280	ml/mol	McGowan Method

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20743504&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):

Legend

chs: Standard solid enthalpy of combustion
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions

hvap: Enthalpy of vaporization at standard conditions

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume