6H-Pyrazolo[1,2-a][1,2,4,5]tetrazine, hexahydro-2,3-dimethyl-

Inchi: InChI=1S/C7H16N4/c1-8-6-10-4-3-5-11(10)7-9(8)2/h3-7H2,1-2H3
InchiKey: ZXYGCFBABNUHAS-UHFFFAOYSA-N
Formula: C7H16N4
SMILES: CN1CN2CCCN2CN1C
Mol. weight [g/mol]: 156.23
CAS: 70517-50-9

Physical Properties

Property code	Value	Unit	Source
ie	7.76	eV	NIST Webbook
log10ws	0.21		Crippen Method
logp	-0.384		Crippen Method
mcvol	127.690	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C70517509&Units=SI
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

Legend

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.