

1H,5H,7H,11H-Dipyrazolo[1,2-a:1',2'-d][1,2,4,5]tetrahydro-

InChI=1S/C8H16N4/c1-3-9-7-11-5-2-6-12(11)8-10(9)4-1/h1-8H2
InChIKey: GGZMLDGVQLXDL-D-UHFFFAOYSA-N
Formula: C8H16N4
SMILES: C1CN2CN3CCCN3CN2C1
Mol. weight [g/mol]: 168.24
CAS: 37882-92-1

Physical Properties

Property code	Value	Unit	Source
ie	7.55	eV	NIST Webbook
log10ws	-0.11		Crippen Method
logp	-0.240		Crippen Method
mvol	130.920	ml/mol	McGowan Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C37882921&Units=SI>

Legend

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

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