1-METHYL-5-NITROPYRAZOLE

Inchi: InChI=1S/C4H5N3O2/c1-6-4(7(8)9)2-3-5-6/h2-3H,1H3
InchiKey: COVPJOWITGLAKX-UHFFFAOYSA-N
Formula: C4H5N3O2
SMILES: Cn1nccc1[N+](=O)[O-]
Mol. weight [g/mol]: 127.10

Physical Properties

Property code	Value	Unit	Source
affp	850.30	kJ/mol	NIST Webbook
basg	818.40	kJ/mol	NIST Webbook
logp	0.328		Crippen Method
mcvol	85.140	ml/mol	McGowan Method

Sources

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):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C54210332&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

affp: Proton affinity
basg: Gas basicity
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume