

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
CAS: 54210-33-2

Physical Properties

Property code	Value	Unit	Source
affp	850.30	kJ/mol	NIST Webbook
basg	818.40	kJ/mol	NIST Webbook
log10ws	-3.18		Crippen Method
logp	0.328		Crippen Method
mcvol	85.140	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=C54210332&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp: Proton affinity
basg: Gas basicity
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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