1-Methyl-3-nitropyrazole

Inchi: InChI=1S/C4H5N3O2/c1-6-3-2-4(5-6)7(8)9/h2-3H,1H3
InchiKey: KLAQNTBUXCCZHC-UHFFFAOYSA-N
Formula: C4H5N3O2
SMILES: Cn1ccc([N+](=O)[O-])n1
Mol. weight [g/mol]: 127.10
CAS: 54210-32-1

Physical Properties

Property code	Value	Unit	Source
affp	847.60	kJ/mol	NIST Webbook
basg	815.70	kJ/mol	NIST Webbook
log10ws	-3.18		Crippen Method
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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C54210321&Units=SI

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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