1H-Pyrazole, 4-nitro-

Other names:	4-NO2-pyrazole
	4-nitro-1H-pyrazole
	4-nitropyrazole
	Pyrazole, 4-nitro-
Inchi:	InChI=1S/C3H3N3O2/c7-6(8)3-1-4-5-2-3/h1-2H,(H,4,5)
InchiKey:	XORHNJQEWQGXCN-UHFFFAOYSA-N
Formula:	C3H3N3O
SMILES:	O=[N+]([O-])c1cn[nH]c1
Mol. weight [g/mol]:	97.08
CAS:	2075-46-9

Physical Properties

Property code	Value	Unit	Source
affp	822.20	kJ/mol	NIST Webbook
basg	788.70	kJ/mol	NIST Webbook
log10ws	-1.11		Crippen Method
logp	-0.164		Crippen Method
mcvol	71.050	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Determination and thermodynamic modelling for 4-nitropyrazole solubility in (methanol + water), (ethanol + water) and (acetonitrile + water) binary solvent mixtures from T = (278.15 to 318.15) K:	https://www.doi.org/10.1016/j.jct.2016.08.023
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2075469&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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