3,5-Dinitro-1H-pyrazole

Other names: 3,5-dinitropyrazole
Inchi: InChI=1S/C3H2N4O4/c8-6(9)2-1-3(5-4-2)7(10)11/h1H,(H,4,5)
InchiKey: UKZXCZWGGXVKNN-UHFFFAOYSA-N
Formula: C3H2N4O4
SMILES: O=[N+]([O-])c1cc([N+](=O)[O-])[nH]n1
Mol. weight [g/mol]: 158.07
CAS: 38858-89-8

Physical Properties

Property code	Value	Unit	Source
affp	759.40	kJ/mol	NIST Webbook
basg	727.50	kJ/mol	NIST Webbook
log10ws	-1.76		Crippen Method
logp	-0.256		Crippen Method
mcvol	88.470	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=C38858898&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