

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/ci9903071
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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