1-methyl-3,5-dinitropyrazole

Inchi: InChI=1S/C4H4N4O4/c1-6-4(8(11)12)2-3(5-6)7(9)10/h2H,1H3
InchiKey: UWSPNIADTGDCIW-UHFFFAOYSA-N
Formula: C4H4N4O4
SMILES: Cn1nc([N+](=O)[O-])cc1[N+](=O)[O-]
Mol. weight [g/mol]: 172.10
CAS: 32683-48-0

Physical Properties

Property code	Value	Unit	Source
affp	788.80	kJ/mol	NIST Webbook
basg	757.00	kJ/mol	NIST Webbook
log10ws	-3.83		Crippen Method
logp	0.236		Crippen Method
mcvol	102.560	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=C32683480&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

Latest version available from: