3-Cyano-5-(cyanofurazanyl)-1,2,4-oxadiazole N-oxide

Inchi: InChI=1S/C6N6O3/c7-1-3-5(11-15-12(3)13)6-9-4(2-8)10-14-6
InchiKey: KMADKHVJAMSJAL-UHFFFAOYSA-N
Formula: C6N6O3
SMILES: N#Cc1noc(-c2no[n+]([O-])c2C#N)n1
Mol. weight [g/mol]: 204.10
CAS: 56092-91-2

Physical Properties

Property code	Value	Unit	Source
chs	-2926.00 ± 4.20	kJ/mol	NIST Webbook
hfs	565.30 ± 4.20	kJ/mol	NIST Webbook
log10ws	-13.07		Crippen Method
logp	-0.899		Crippen Method
mcvol	116.770	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C56092912&Units=SI
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

Legend

chs: Standard solid enthalpy of combustion
hfs: Solid phase enthalpy of formation at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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