2-Furoic acid, 5-nitro-,anhydride

Inchi: InChI=1S/C10H4N2O9/c13-9(5-1-3-7(19-5)11(15)16)21-10(14)6-2-4-8(20-6)12(17)18/h1-
InchiKey: AUKYKYFQJGYKJN-UHFFFAOYSA-N
Formula: C10H4N2O9
SMILES: O=C(OC(=O)c1ccc([N+](=O)[O-])o1)c1ccc([N+](=O)[O-])o1
Mol. weight [g/mol]: 296.15
CAS: 33794-66-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.45		Crippen Method
logp	1.686		Crippen Method
mcvol	168.430	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=C33794660&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume