

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/ci9903071
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

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