2-Acetyl-5-nitrobenzo[b]furan

Inchi: InChI=1S/C10H7NO4/c1-6(12)10-5-7-4-8(11(13)14)2-3-9(7)15-10/h2-5H,1H3
InchiKey: RMXFQPLULZFJMH-UHFFFAOYSA-N
Formula: C10H7NO4
SMILES: CC(=O)c1cc2cc([N+](=O)[O-])ccc2o1
Mol. weight [g/mol]: 205.17
CAS: 23136-39-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.32		Crippen Method
logp	2.544		Crippen Method
mcvol	137.700	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=C23136392&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