

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:	RMXFQPLULZFMH-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

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