3-Acetoxybenzofuran

Inchi: InChI=1S/C10H8O3/c1-7(11)13-10-6-12-9-5-3-2-4-8(9)10/h2-6H,1H3
InchiKey: XCBLZAJCKKRBED-UHFFFAOYSA-N
Formula: C10H8O3
SMILES: CC(=O)Oc1coc2ccccc12
Mol. weight [g/mol]: 176.17
CAS: 93680-80-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.32		Crippen Method
logp	2.358		Crippen Method
mcvol	126.150	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=C93680809&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