

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/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

Latest version available from:

<https://www.chemeo.com/cid/55-736-4/3-Acetoxybenzofuran.pdf>

Generated by Cheméo on 2024-04-29 22:10:06.592095794 +0000 UTC m=+16717855.512673105.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.