5-Acetoxymethyl-2-furaldehyde

Other names: 2-Furancarboxaldehyde, 5-[(acetyloxy)methyl]-
5-Acetoxymethylfurfural
5-formylfurfuryl acetate
Inchi: InChI=1S/C8H8O4/c1-6(10)11-5-8-3-2-7(4-9)12-8/h2-4H,5H2,1H3
InchiKey: QAVITTVTXPZTSE-UHFFFAOYSA-N
Formula: C8H8O4
SMILES: CC(=O)OCc1ccc(C=O)o1
Mol. weight [g/mol]: 168.15
CAS: 10551-58-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.03		Crippen Method
logp	1.155		Crippen Method
mcvol	119.000	ml/mol	McGowan Method
rinpol	1304.10		NIST Webbook
rinpol	1304.10		NIST Webbook
ripol	2199.00		NIST Webbook
ripol	2176.00		NIST Webbook
ripol	2194.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10551583&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws: Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices