

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/ci990307I
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

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