

5-Methylfurfuryl acetate

Other names: 5-formyl-2-furfurylethanoate
Inchi: InChI=1S/C8H10O3/c1-6-3-4-8(11-6)5-10-7(2)9/h3-4H,5H2,1-2H3
InchiKey: WCAYUXKMYBPHIN-UHFFFAOYSA-N
Formula: C8H10O3
SMILES: CC(=O)OCc1ccc(C)o1
Mol. weight [g/mol]: 154.16
CAS: 18091-24-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.26		Crippen Method
logp	1.651		Crippen Method
mcvol	117.430	ml/mol	McGowan Method
ripol	2194.00		NIST Webbook
ripol	2194.00		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C18091242&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
ripol: Polar retention indices

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