5-formyl-2-furfurylmethanoate

Inchi: InChI=1S/C7H8O3/c1-6-2-3-7(10-6)4-9-5-8/h2-3,5H,4H2,1H3
InchiKey: UJIYLTWAHDYJDZ-UHFFFAOYSA-N
Formula: C7H8O3
SMILES: Cc1ccc(COC=O)o1
Mol. weight [g/mol]: 140.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.84		Crippen Method
logp	1.261		Crippen Method
mcvol	103.340	ml/mol	McGowan Method
ripol	2183.00		NIST Webbook
ripol	2183.00		NIST Webbook

Sources

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=R492861&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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