1-(3-furfuryl)pyrrole-2-carboxaldehyde

Inchi: InChI=1S/C10H9NO2/c12-7-10-2-1-4-11(10)6-9-3-5-13-8-9/h1-5,7-8H,6H2
InchiKey: PQJSXBOAVGKEMP-UHFFFAOYSA-N
Formula: C10H9NO2
SMILES: O=Cc1cccn1Cc1ccoc1
Mol. weight [g/mol]: 175.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.01		Crippen Method
logp	1.942		Crippen Method
mcvol	130.260	ml/mol	McGowan Method
rinpol	1399.00		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=R230316&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices