

N-furfuryl-2-formylpyrrole

Inchi: InChI=1S/C9H7NO2/c11-7-8-3-1-5-10(8)9-4-2-6-12-9/h1-7H
InchiKey: KTQWSUVONDQZBG-UHFFFAOYSA-N
Formula: C9H7NO2
SMILES: O=Cc1cccn1-c1cco1
Mol. weight [g/mol]: 161.16

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.10		Crippen Method
logp	1.883		Crippen Method
mcvol	116.170	ml/mol	McGowan Method
rinpol	1345.00		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=R225106&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

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<https://www.chemeo.com/cid/20-039-6/N-furfuryl-2-formylpyrrole.pdf>

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