2-Furancarbaldehyde

Inchi: InChI=1S/C5H4O2/c6-4-5-2-1-3-7-5/h1-4H
InchiKey: HYBBIBNJHNGZAN-UHFFFAOYSA-N
Formula: C5H4O2
SMILES: O=Cc1ccco1
Mol. weight [g/mol]: 96.08

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.45		Crippen Method
logp	1.092		Crippen Method
mcvol	69.290	ml/mol	McGowan Method
ripol	1425.00		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=R599774&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