

Furfural oxime

Inchi: InChI=1S/C5H5NO2/c7-6-4-5-2-1-3-8-5/h1-4,7H
InchiKey: UYTMLDBQFLIQJA-UHFFFAOYSA-N
Formula: C5H5NO2
SMILES: ON=Cc1ccco1
Mol. weight [g/mol]: 111.10
CAS: 1121-47-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.51		Crippen Method
logp	1.088		Crippen Method
mcvol	79.270	ml/mol	McGowan Method
rinpol	1048.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1121477&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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.cheméo.com/cid/53-175-9/Furfural-oxime.pdf>

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