3-formyl-2-methylfuran

Inchi: InChI=1S/C6H6O2/c1-5-6(4-7)2-3-8-5/h2-4H,1H3
InchiKey: WBFUBNWKSDINIX-UHFFFAOYSA-N
Formula: C6H6O2
SMILES: Cc1occc1C=O
Mol. weight [g/mol]: 110.11

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.92		Crippen Method
logp	1.401		Crippen Method
mcvol	83.380	ml/mol	McGowan Method
rinpol	931.00		NIST Webbook
rinpol	931.00		NIST Webbook
rinpol	936.00		NIST Webbook
rinpol	936.00		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=R495355&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

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