3-Formyl-1-methylpyrrole

Inchi: InChI=1S/C6H7NO/c1-7-3-2-6(4-7)5-8/h2-5H,1H3
InchiKey: OXADKJPOZQYWIG-UHFFFAOYSA-N
Formula: C6H7NO
SMILES: Cn1ccc(C=O)c1
Mol. weight [g/mol]: 109.13

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.00		Crippen Method
logp	0.838		Crippen Method
mcvol	87.490	ml/mol	McGowan Method
ripol	2012.00		NIST Webbook
ripol	2012.00		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=R517970&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
ripol: Polar retention indices

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