

1,2-Dimethylpyridone

Inchi: InChI=1S/C7H9NO/c1-6-5-7(9)3-4-8(6)2/h3-5H,1-2H3
InchiKey: KHHWWVUYCPMGEL-UHFFFAOYSA-N
Formula: C7H9NO
SMILES: Cc1cc(=O)ccn1C
Mol. weight [g/mol]: 123.15

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.66		Crippen Method
logp	0.694		Crippen Method
mcvol	101.580	ml/mol	McGowan Method
ripol	1611.00		NIST Webbook
ripol	1611.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R519025&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
ripol: Polar retention indices

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