N-Formylloline

Inchi: InChI=1S/C9H14N2O2/c1-10(5-12)8-7-4-11-3-2-6(13-7)9(8)11/h5-9H,2-4H2,1H3/t6-,7+,8
InchiKey: YHLKXYXFUCTURZ-OBCZXFEGSA-N
Formula: C9H14N2O2
SMILES: CN(C=O)C1C2CN3CCC(O2)C13
Mol. weight [g/mol]: 182.22

Physical Properties

Property code	Value	Unit	Source
log10ws	0.28		Crippen Method
logp	-0.702		Crippen Method
mcvol	132.490	ml/mol	McGowan Method
rinpol	1600.00		NIST Webbook
rinpol	1603.00		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=R268321&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
rinpol: Non-polar retention indices

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