1-Piperidinecarboxaldehyde, 2-(3,4-dihydro-2H-pyrrol-5-yl)-

Other names: Smipine
Inchi: InChI=1S/C10H16N2O/c13-8-12-7-2-1-5-10(12)9-4-3-6-11-9/h8,10H,1-7H2
InchiKey: FBNJGSJNODLRSZ-UHFFFAOYSA-N
Formula: C10H16N2O
SMILES: O=CN1CCCCC1C1=NCCC1
Mol. weight [g/mol]: 180.25
CAS: 52196-11-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.42		Crippen Method
logp	1.232		Crippen Method
mcvol	147.270	ml/mol	McGowan Method
rinpol	1580.00		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=C52196119&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