3-(5-methylfurfurylidene)-1-pyrroline, (Z)

Inchi: InChI=1S/C10H11NO/c1-8-2-3-10(12-8)6-9-4-5-11-7-9/h2-3,6-7H,4-5H2,1H3/b9-6-
InchiKey: BCWSVRKZMCXABS-TWGQIWQCSA-N
Formula: C10H11NO
SMILES: Cc1ccc(C=C2C=NCC2)o1
Mol. weight [g/mol]: 161.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.82		Crippen Method
logp	2.446		Crippen Method
mcvol	128.690	ml/mol	McGowan Method
ripol	2128.00		NIST Webbook
ripol	2128.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R315343&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.