

3-furfurylidene pyrrolidine

Inchi: InChI=1S/C9H11NO/c1-2-9(11-5-1)6-8-3-4-10-7-8/h1-2,5-6,10H,3-4,7H2/b8-6-
InchiKey: PNXYWYJGINUMYJQ-VURMDHGXSA-N
Formula: C9H11NO
SMILES: C(=C1CCNC1)c1ccco1
Mol. weight [g/mol]: 149.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.37		Crippen Method
logp	1.656		Crippen Method
mcvol	118.900	ml/mol	McGowan Method
ripol	2045.00		NIST Webbook
ripol	2050.00		NIST Webbook
ripol	2045.00		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=R315254&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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<https://www.chemeo.com/cid/81-458-4/3-furfurylidene-pyrrolidine.pdf>

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