

1-[3-(methylthio)propyl]-2-formylpyrrole

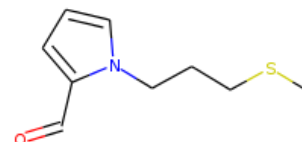
InChI: InChI=1S/C9H13NOS/c1-12-7-3-6-10-5-2-4-9(10)8-11/h2,4-5,8H,3,6-7H2,1H3

InChI Key: POEWGUCPJZNVBU-UHFFFAOYSA-N

Formula: C9H13NOS

SMILES: CSCCCn1cccc1C=O

Molecular Weight: 183.27



Physical Properties

Property	Value	Unit	Source
$\log P_{\text{oct/wat}}$	2.05		Crippen Method

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C9H13NOS/c1-12-7-3-6-10-5-2-4-9\(10\)8-11/h2,4-5,8H,3,6-7H2,1H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C9H13NOS/c1-12-7-3-6-10-5-2-4-9(10)8-11/h2,4-5,8H,3,6-7H2,1H3)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$\log P_{\text{oct/wat}}$: Octanol/Water partition coefficient .

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