

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
InchiKey:	POEWGUCPJZNVBU-UHFFFAOYSA-N
Formula:	C9H13NOS
SMILES:	CSCCCn1cccc1C=O
Mol. weight [g/mol]:	183.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.70		Crippen Method
logp	2.054		Crippen Method
mcvol	146.110	ml/mol	McGowan Method
rinpola	1504.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U366010&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices

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