

1-(Methylthio)propylpyrrole

Inchi: InChI=1S/C8H13NS/c1-10-8-4-7-9-5-2-3-6-9/h2-3,5-6H,4,7-8H2,1H3
InchiKey: UMRWNUKKSKEHP-UHFFFAOYSA-N
Formula: C8H13NS
SMILES: CSCCCn1cccc1
Mol. weight [g/mol]: 155.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.45		Crippen Method
logp	2.241		Crippen Method
mcvol	130.450	ml/mol	McGowan Method
ripol	1950.00		NIST Webbook
ripol	1950.00		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R319667&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
ripol: Polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/91-774-2/1-Methylthio-propylpyrrole.pdf>

Generated by Cheméo on 2024-04-23 13:17:52.683205629 +0000 UTC m=+16167521.603782944.

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