2-pyrrolemethyl thioacetate

Inchi: InChI=1S/C7H9NOS/c1-6(9)10-5-7-3-2-4-8-7/h2-4,8H,5H2,1H3
InchiKey: MBBCEIDZMLKQAB-UHFFFAOYSA-N
Formula: C7H9NOS
SMILES: CC(=O)SCc1ccc[nH]1
Mol. weight [g/mol]: 155.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.07		Crippen Method
logp	1.312		Crippen Method
mcvol	117.930	ml/mol	McGowan Method
ripol	2293.00		NIST Webbook
ripol	2293.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R336404&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.