1H-pyrrolo[2,1-c]-1,4-thiazine

Inchi: InChI=1S/C7H7NS/c1-2-7-6-9-5-4-8(7)3-1/h1-5H,6H2
InchiKey: LMFZCLWJOUSWGP-UHFFFAOYSA-N
Formula: C7H7NS
SMILES: C1=Cn2cccc2CS1
Mol. weight [g/mol]: 137.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.91		Crippen Method
logp	2.163		Crippen Method
mcvol	101.200	ml/mol	McGowan Method
rinpol	1226.00		NIST Webbook
ripol	1977.00		NIST Webbook
ripol	1977.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R169145&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
rinpol: Non-polar retention indices
ripol: Polar retention indices

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