Cyclopentathiazole

Inchi: InChI=1S/C6H7NS/c1-2-5-6(3-1)8-4-7-5/h4H,1-3H2
InchiKey: QCCKBDNIBZPFCH-UHFFFAOYSA-N
Formula: C6H7NS
SMILES: c1nc2c(s1)CCC2
Mol. weight [g/mol]: 125.19
CAS: 5661-10-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.08		Crippen Method
logp	1.632		Crippen Method
mcvol	91.410	ml/mol	McGowan Method
ripol	1551.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5661109&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
ripol: Polar retention indices

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