2-methyl-5,7-dihydrothieno[3,4-d]pyrimidine

Inchi: InChI=1S/C7H8N2S/c1-5-8-2-6-3-10-4-7(6)9-5/h2H,3-4H2,1H3
InchiKey: XSUYIZJJKIKWFN-UHFFFAOYSA-N
Formula: C7H8N2S
SMILES: Cc1ncc2c(n1)CSC2
Mol. weight [g/mol]: 152.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.02		Crippen Method
logp	1.532		Crippen Method
mcvol	111.180	ml/mol	McGowan Method
rinpol	1339.00		NIST Webbook
rinpol	1339.00		NIST Webbook
ripol	2137.00		NIST Webbook

Sources

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=R169254&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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