pyrrolidino[1,2-e]-4H-2,4-dimethyl-1,3,5-dithiazine

Other names: Pyrrolidino[1,2-e]-4H-1,3,5-dithiazine, 2,4-dimethyl
Inchi: InChI=1S/C8H15NS2/c1-6-9-5-3-4-8(9)11-7(2)10-6/h6-8H,3-5H2,1-2H3
InchiKey: OJEOXDLLIADRBL-UHFFFAOYSA-N
Formula: C8H15NS2
SMILES: CC1SC(C)N2CCCC2S1
Mol. weight [g/mol]: 189.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.12		Crippen Method
logp	2.580		Crippen Method
mcvol	144.540	ml/mol	McGowan Method
rinpol	1462.00		NIST Webbook
rinpol	1462.00		NIST Webbook
rinpol	1462.00		NIST Webbook
ripol	1990.00		NIST Webbook
ripol	1990.00		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=R62449&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