Pyrrolidino[1,2-e]-4H-1,3,5-dithiazine, 4-methyl-2-propyl

Inchi: InChI=1S/C10H19NS2/c1-3-5-10-12-8(2)11-7-4-6-9(11)13-10/h8-10H,3-7H2,1-2H3
InchiKey: CUMZZYRQJYRZDG-UHFFFAOYSA-N
Formula: C10H19NS2
SMILES: CCCC1SC(C)N2CCCC2S1
Mol. weight [g/mol]: 217.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.96		Crippen Method
logp	3.361		Crippen Method
mcvol	172.720	ml/mol	McGowan Method
rinpol	1621.00		NIST Webbook
rinpol	1621.00		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=R62467&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.