Pyrrolidino[1,2-e]-4H-1,3,5-dithiazine, 4-methyl-2-(2-methylpropyl)

Inchi: InChI=1S/C11H21NS2/c1-8(2)7-11-13-9(3)12-6-4-5-10(12)14-11/h8-11H,4-7H2,1-3H3
InchiKey: KQKAMJHDZLMOPY-UHFFFAOYSA-N
Formula: C11H21NS2
SMILES: CC(C)CC1SC(C)N2CCCC2S1
Mol. weight [g/mol]: 231.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.13		Crippen Method
logp	3.607		Crippen Method
mcvol	186.810	ml/mol	McGowan Method
rinpol	1703.00		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=R62453&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