Pyrrolidino[1,2-e]-4H-1,3,5-dithiolane, 2-butyl-4-methyl

Inchi: InChI=1S/C11H21NS2/c1-3-4-7-11-13-9(2)12-8-5-6-10(12)14-11/h9-11H,3-8H2,1-2H3
InchiKey: NCUIAOPINFJUBZ-UHFFFAOYSA-N
Formula: C11H21NS2
SMILES: CCCCC1SC(C)N2CCCC2S1
Mol. weight [g/mol]: 231.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.37		Crippen Method
logp	3.751		Crippen Method
mcvol	186.810	ml/mol	McGowan Method
rinpol	1723.00		NIST Webbook
rinpol	1723.00		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=R62471&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.