Triazolo [4,5-d]pyrimidine-,3h-v-,7(6h)-thione-, 5-amino-3-butyl-

Inchi: InChI=1S/C8H12N6S/c1-2-3-4-14-6-5(12-13-14)7(15)11-8(9)10-6/h2-4H2,1H3,(H3,9,10,1

InchiKey: CFGHKHQFYJJBHW-UHFFFAOYSA-N

Formula: C8H12N6S

SMILES: CCCCn1nnc2c(=S)[nH]c(N)nc21

Mol. weight [g/mol]: 224.29

CAS: 92352-41-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.38		Crippen Method
logp	0.784		Crippen Method
mcvol	160.890	ml/mol	McGowan Method

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=C92352415&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