

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,(H3,9,10,11)
InchiKey:	CFGHKKHQFYJJBHW-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/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/56-936-1/Triazolo-4-5-d-pyrimidine-3h-v-7-6h-thione-5-amino-3-butyl.pdf>

Generated by Cheméo on 2024-05-21 19:23:29.14226621 +0000 UTC m=+18608658.062843520.

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