

[1,2,5]Thiadiazolo[3,4-d]pyrimidine, 5-amino-7-butylamino-

Inchi:	InChI=1S/C8H12N6S/c1-2-3-4-10-6-5-7(14-15-13-5)12-8(9)11-6/h2-4H2,1H3,(H3,9,10,11)
InchiKey:	GXCZMRDVTTHOASY-UHFFFAOYSA-N
Formula:	C8H12N6S
SMILES:	CCCCNc1nc(N)nc2nsnc12
Mol. weight [g/mol]:	224.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.99		Crippen Method
logp	1.276		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=B6008427&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/66-521-0/1-2-5-Thiadiazolo-3-4-d-pyrimidine-5-amino-7-butylamino.pdf>

Generated by Cheméo on 2024-04-25 22:16:50.871768311 +0000 UTC m=+16372659.792345624.

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