

4-Amino-n-butyl-1,2,5-thiadiazole-3-carboximidam

Inchi:	InChI=1S/C7H13N5S/c1-2-3-4-10-6(8)5-7(9)12-13-11-5/h2-4H2,1H3,(H2,8,10)(H2,9,12)
InchiKey:	JQFOWNKCLKWBOT-UHFFFAOYSA-N
Formula:	C7H13N5S
SMILES:	CCCCNC(=N)c1nsnc1N
Mol. weight [g/mol]:	199.28
CAS:	7501-30-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.15		Crippen Method
logp	0.835		Crippen Method
mcvol	151.980	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7501306&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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