

1,2,5-Thiadiazole, 3-(n-butylcarbamoyl)-4-ureido-

Inchi:	InChI=1S/C8H13N5O2S/c1-2-3-4-10-7(14)5-6(11-8(9)15)13-16-12-5/h2-4H2,1H3,(H,10,11)
InchiKey:	IADZSJMFQQNWDQ-UHFFFAOYSA-N
Formula:	C8H13N5O2S
SMILES:	CCCCNC(=O)c1nsnc1NC(N)=O
Mol. weight [g/mol]:	243.29
CAS:	7501-18-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.56		Crippen Method
logp	0.559		Crippen Method
mcvol	173.510	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=C7501180&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

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