

2-Oxazolidinone, n-[2-(2-pyridylthio)ethyl]-

Inchi:	InChI=1S/C10H12N2O2S/c13-10-12(5-7-14-10)6-8-15-9-3-1-2-4-11-9/h1-4H,5-8H2
InchiKey:	PMVRWBAJZBHGIR-UHFFFAOYSA-N
Formula:	C10H12N2O2S
SMILES:	O=C1OCCN1CCSc1ccccn1
Mol. weight [g/mol]:	224.28
CAS:	22280-16-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.96		Crippen Method
logp	1.626		Crippen Method
mcvol	160.890	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C22280166&Units=SI

Legend

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

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