

3-Phenyl-2-oxazolidinone

Inchi:	InChI=1S/C9H9NO2/c11-9-10(6-7-12-9)8-4-2-1-3-5-8/h1-5H,6-7H2
InchiKey:	NCTCGHLIHJJIBK-UHFFFAOYSA-N
Formula:	C9H9NO2
SMILES:	O=C1OCCN1c1ccccc1
Mol. weight [g/mol]:	163.17
CAS:	703-56-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.53		Crippen Method
logp	1.643		Crippen Method
mcvol	120.470	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C703560&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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<https://www.chemeo.com/cid/60-685-5/3-Phenyl-2-oxazolidinone.pdf>

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