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