2-Benzothiazolinone, 3-methyl-

Inchi: InChI=1S/C8H7NOS/c1-9-6-4-2-3-5-7(6)11-8(9)10/h2-5H,1H3
InchiKey: LSMMRJUHLKJNLR-UHFFFAOYSA-N
Formula: C8H7NOS
SMILES: Cn1c(=O)sc2ccccc21
Mol. weight [g/mol]: 165.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.74		Crippen Method
logp	1.600		Crippen Method
mcvol	116.860	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=B6005289&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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