Acetoacetamide, n-(2-benzothiazolyl)-

Inchi: InChI=1S/C11H10N2O2S/c1-7(14)6-10(15)13-11-12-8-4-2-3-5-9(8)16-11/h2-5H,6H2,1H3
InchiKey: KRVAVIMTIIEASB-UHFFFAOYSA-N
Formula: C11H10N2O2S
SMILES: CC(=O)CC(=O)Nc1nc2ccccc2s1
Mol. weight [g/mol]: 234.27
CAS: 4692-94-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.12		Crippen Method
logp	2.214		Crippen Method
mcvol	166.380	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=C4692948&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