

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:	KRVAVIMTIIIEASB-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/ci9903071
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

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<https://www.chemeo.com/cid/117-583-5/Acetoacetamide-n-2-benzothiazolyl.pdf>

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