

Ethanone, 1-(2-benzothiazolyl)-

Inchi:	InChI=1S/C9H7NOS/c1-6(11)9-10-7-4-2-3-5-8(7)12-9/h2-5H,1H3
InchiKey:	GSTOPVVGJHLPSBJ-UHFFFAOYSA-N
Formula:	C9H7NOS
SMILES:	CC(=O)c1nc2ccccc2s1
Mol. weight [g/mol]:	177.22
CAS:	1629-78-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.46		Crippen Method
logp	2.499		Crippen Method
mcvol	126.650	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=C1629783&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

Latest version available from:

<https://www.chemeo.com/cid/19-242-2/Ethanone-1-2-benzothiazolyl.pdf>

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