

Oxime of 5-acetyl-4-methyl-4-thiazoline-2-thione

Inchi:	InChI=1S/C6H8N2OS2/c1-3-5(4(2)8-9)11-6(10)7-3/h9H,1-2H3,(H,7,10)/b8-4+
InchiKey:	ZFYHJVSPWMVAQL-XBXARRHUSA-N
Formula:	C6H8N2OS2
SMILES:	CC(=NO)c1sc(=S)[nH]c1C
Mol. weight [g/mol]:	188.27
CAS:	89691-87-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.50		Crippen Method
logp	1.830		Crippen Method
mcvol	130.170	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=C89691872&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

Latest version available from:

<https://www.chemeo.com/cid/51-193-1/Oxime-of-5-acetyl-4-methyl-4-thiazoline-2-thione.pdf>

Generated by Cheméo on 2024-05-16 06:00:50.052347271 +0000 UTC m=+18128498.972924588.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.