

2-Acetyl-5-cyanothiophene

Inchi:	InChI=1S/C7H5NOS/c1-5(9)7-3-2-6(4-8)10-7/h2-3H,1H3
InchiKey:	VSHPLUBHIUFLES-UHFFFAOYSA-N
Formula:	C7H5NOS
SMILES:	CC(=O)c1ccc(C#N)s1
Mol. weight [g/mol]:	151.19
CAS:	88653-55-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.24		Crippen Method
logp	1.822		Crippen Method
mcvol	109.330	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C88653558&Units=SI

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/65-442-9/2-Acetyl-5-cyanothiophene.pdf>

Generated by Cheméo on 2025-12-23 09:49:16.841742317 +0000 UTC m=+6231554.371782971.

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