

2-Acetyl-3-aminothiophene

Inchi:	InChI=1S/C6H7NOS/c1-4(8)5-2-3-6(7)9-5/h2-3H,7H2,1H3
InchiKey:	ZCNRCSLSOFXYL-LUHFFFAOYSA-N
Formula:	C6H7NOS
SMILES:	CC(=O)c1ccc(N)s1
Mol. weight [g/mol]:	141.19
CAS:	31968-33-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.52		Crippen Method
logp	1.533		Crippen Method
mcvol	103.840	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C31968339&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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