

5-Amino-3-(2-thienyl)pyrazole

Inchi:	InChI=1S/C7H7N3S/c8-7-4-5(9-10-7)6-2-1-3-11-6/h1-4H,(H3,8,9,10)
InchiKey:	TXSOLYKLZBJHFF-UHFFFAOYSA-N
Formula:	C7H7N3S
SMILES:	<chem>Nc1cc(-c2cccs2)n[nH]1</chem>
Mol. weight [g/mol]:	165.22
CAS:	96799-03-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.45		Crippen Method
logp	1.239		Crippen Method
mcvol	116.860	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=C96799030&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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<https://www.chemeo.com/cid/25-737-6/5-Amino-3-2-thienyl-pyrazole.pdf>

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